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ECONOMIC EVALUATION OF WATER QUALITY. A MULTICOMPONENT MODEL OF OPTIMAL QUALITY CONTROL IN ESTUARINE WATERS

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California University
Berkeley, California

January 1969

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A MULTICOMPONENT MODEL OF OPTIMAL QUALITY CONTROL IN ESTUARINE WATERS

Fourth Annual Report

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ECONOMIC EVALUATION OF WATER QUALITY

A MULTICOMPONENT MODEL OF OPTIMAL QUALITY CONTROL IN ESTUARINE WATERS

Fourth Annual Report

by

Shishir K. Mukherjee

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January 1969

Sanitary Engineering Research Laboratory
College of Engineering
and
School of Public Health
University of California
Berkeley

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I. INTRODUCTION

NEED FOR STUDY

During the past few decades, degradation of the environment has created deep public concern and has cast a dark shadow on the bright picture of the affluent society. The purity and the hygienic quality of the air and water resources of the nation are being threatened by increasing pollution, and the quality of life itself is being diminished through a loss of scenic skylines and bodies of water. Unless science and technology, which play the all-important role in our economic prosperity, are directed toward solving these problems of environmental pollution before it is too late, on some future day man may have to consider closing down factories and curtailing his activities for simple physical survival.

The reasons for a mounting interest and concern over pollution problems are concisely expressed in the 1965 report of the Environmental Pollution Panel of the President's Science Advisory Committee.

> The production of pollutants ... are an inevitable concomitant of a technological society with a high standard of living. Pollution problems will increase in importance as our technology and standard of living continues to grow.

Most of the costs and damages due to pollution of streams, lakes, and estuaries are borne by society at large, and often do not greatly affect the pollution-causing agency. As Kneese [1] points out, this introduces "technological external diseconomies" resulting in nonoptimal allocation of resources. The 'market' cannot be trusted to effect sufficient resource allocation into pollution abatement activities, resulting in increased social costs due to pollution. Clearly, there is a need for some better method of dealing with this problem.

CONCEPTS AND RATIONALE

One of the basic objectives of resource management is the optimal allocation of resources. Today it is well recognized that water quality, just as water quantity, should be considered as a natural resource, and one of such scarcity as to justify optimal allocation. However, the basis for appropriate action is not clear. There are very strong arguments that water quality control measures could be justified entirely on economic grounds, presumably using a benefit-cost analysis. The process, however, is extremely difficult because dependable cost-benefit data on water quality do not exist. To be sure, most of the costs of pollution abatement methods are well established, but the social costs of pollution and the benefits of improved water quality are generally intangible. Hence, there is great danger that social costs and benefits may be underestimated and that decisions based on economic grounds alone might endanger even the existence of certain bodies of water by allocating only meager resources to pollution abatement.

The traditional way in which regulatory agencies have sought to deal with the foregoing situation is the "standards" approach which considers the problem of maintaining the quality of a body of water above some minimum value at a cost at least acceptable to the dischargers of wastewater. The value itself, or "standard" [2] is established by a public regulatory agency making use of its own and other available experts. The success of the approach lies in the establishment and maintenance of proper and safe limits of concentration of the various impurities in water deemed worthy of concern. At best it may also seek to achieve its goals at a minimum cost to the region.

It is the underlying rationale of the study herein reported that:

1. Although economic grounds alone are not a sufficient basis for water quality control, the objectives of such control should be attained at a minimum cost.

2. Operations research and systems analysis techniques can be applied to optimizing the cost of achieving water quality objectives.

3. The problem of "technological external diseconomies" noted in the preceding section can be dealt with to an acceptable degree in the case of water quality objectives by internalizing the external diseconomies.

NATURE OF STUDY AND REPORT

Studies of the Economic Evaluation of Water Quality were initiated at the Sanitary Engineering Research Laboratory in 1962. The progress report herein presented is the fourth in a series of "annual" reports released from time to time as individual phases of the study are completed. The First Report, SERL No. 65-3 subtitled "An Engineering-Economic Model for Water Quality Management" [3] was released in January 1965. In it a computer model was developed and applied to a study of the combination of wastewater treatment, natural self-purification, and water treatment processes which would involve the least cost to a group of communities in achieving water resource quality goals for a river subject to various water management schemes and to multiple beneficial uses. The oxygen resource of the stream in terms of dissolved oxygen (DO) was taken as the critical factor governing waste treatment processes. During the study, there was evidence that the normal criteria for DO might prove inadequate. The second phase of the study was therefore directed to the development and testing of a mathematical model expressing the relationship between the oxygen-demanding fractions of a wastewater and the responses of a living stream. Results of this phase of the study were released in the Second Annual Report, SERL No. 65-11 in August 1965, subtitled, "A Mathematical Model of Dissolved Oxygen Concentration in Freshwater Streams." [4]

As domestic, industrial, and agricultural wastewaters may contain various toxic as well as stable chemical compounds, some of which may have adverse effects on human health and marine ecology, a water quality standard with DO as the critical factor is no longer adequate. Instead, a multicomponent water quality parameter is needed in which limiting concentrations of several important water quality constituents express the standard. The need to minimize the cost of achieving any prescribed water goal for a region in any case has been ever present since the beginning of concern for pollution control. The specific objective of study during the third phase, therefore, was to develop, and illustrate by application to an example, a linear programming multicomponent water quality control model capable of minimizing the cost of achieving any given water quality goal when the quantities of various wastes predicted by an input-output model (developed in a parallel project) are reduced to imposed levels by presently known technology. A method of predicting future treatment needs from projections of population and economic growth was also developed as a modification of the model. Results of this phase of the study were released in the Third Annual Report, SERL No. 68-2, in February 1968 under the subtitle, "A Linear Programming Water Quality Control Model." [5]

The fourth phase, herein reported, was initiated in July 1967 while the third phase was still in process. One of the main limitations of the Linear Programming Water Quality Control Model (third phase), reported by Carew and McGauhey [5], is that quality standards are expressed as the maximum allowable quantities of each waste constituent discharged to the water body rather than as the maximum allowable concentration levels in the water resource itself. The fourth phase seeks to remove this limitation by the development of Dispersion Models for optimal allocation of water quality and integration of a dispersion model with the model of water quality control reported by Carew and McGauhey.

Although the final model is developed with reference to an estuary, it is regional in nature and applicable to a river system terminating in an estuary. In fact, the whole river basin, including the estuary and the waste-producing activities within it, is considered to be in one "system." The model becomes a device for generating an optimal plan of effluent treatment and discharge which minimizes the total treatment cost in the estuarine basin on the basis of data inputs on:

1. Acceptable water quality, expressed at maximum allowable concentrations of important quality constituents in the estuary,
2. hydrology of the estuary,
3. location, quantities, and compositions of waste effluents generated by various industries and municipalities in the estuarine basin,
4. technology and economics of available waste treatment processes.

If social costs of pollution are known or evaluated, these also could be included in the model.

Specifically, an optimization model is presented, based on a one-dimensional description of the dispersion process which includes both longitudinal dispersion and advection in an estuary. It can be used for an estuary where tidal effects are pronounced and downstream velocity is low, or for a fast-flowing river.

A steady state model is described in detail for quality conditions averaged over a tidal cycle. To include seasonal variations of volume flow rate, waste generation and discharge rates, and other hydrological parameters, an unsteady state model was developed.

If projections of future population and industrial growth are available, giving an estimate of future waste loads, the model may be used to obtain future plans for water quality control and to ascertain needs for future investments. Various alternative quality standards could be evaluated in terms of their optimal cost to obtain a quality-cost surface. Such information would be very valuable for regional or governmental authorities in prescribing quality standards and finance quality-improvement projects.

The model envisages the establishment of a regional organization for management of the optimal control plan and for equitable distribution of treatment costs among the various polluting agencies. It also suggests the establishment of a system of charges or taxes for the polluting agencies based on the quantity and composition of their effluent discharge. The rates of such charges are obtained as dual prices in the model, and are helpful for equitable distribution of costs among polluting agencies.

OBJECTIVES OF STUDY

The overall objectives of the study, beyond those of the third phase, were to utilize the techniques of operations research to determine the economic effects of changing the water quality requirements of an estuarine water basin.

The specific objectives were:

1. To study the transportation, dispersion, and degradation of waste constituents in an estuarine basin, aimed at relating the resulting concentration to the amounts and locations of waste discharges and hydrological parameters.
2. To develop dispersion models for optimal allocation of water quality in an estuary to achieve various related objectives, and solution of the continuous versions of these models by the application of optimal control theory to obtain an insight into the nature of optimal discharge policies.

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3. To develop discrete versions of the dispersion models as linear programs, with a view to using the discrete data available from sampling studies in an estuary.

4. To develop an integrated multicomponent model of dispersion and waste treatment which will simultaneously provide an optimal plan of waste treatment, along with a plan of optimal waste discharge along the estuary, given a prescribed quality standard, and solve it as a linear program.

5. To study various modifications of the model and the economic effects of various alternative quality-improvement projects, such as flow augmentation and transportation of waste by piping within the estuary or directly to the ocean.

ORGANIZATION FOR STUDY

The study was conducted by the Sanitary Engineering Research Laboratory (SERL) of the University of California under Grant No. USDI WP-597 from the Federal Water Pollution Control Administration. Professor P. H. McGauhey, Director of SERL, served as Faculty Investigator for the study. Research and investigative work was performed by Mr. Shishir Kumar Mukherjee, Junior Specialist, and project leader.

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II. THE DISPERSION MODEL

INTRODUCTION

The first step in generating a model for estuarine water quality management is the development of a "Dispersion Model." It aims at the optimum use of water resources for waste disposal purposes by maximizing the total amount of each of the various pollutants discharged, while maintaining a specified acceptable level of quality in the estuarine body of water. The dispersion model in conjunction with the waste treatment model (Chapter VI) generates an optimal plan of effluent treatment and discharge, by minimizing the total pollution abatement costs for the estuarine basin.

SUMMARY OF MIXING, DISPERSION, AND DECAYING PROCESSES IN ESTUARIES

Transportation of soluble or colloidal polluting substances discharged into a body of water, and the subsequent mixing, may be considered as two distinct processes which occur simultaneously. Depending on the hydrology of the particular stream, lake, or estuary, either of these processes may become dominant over the other.

Advection (Plug Flow)

Polluting substances in solution or mixed state are carried downstream by advection with the same velocity as that of the flowing water. For fast-flowing rivers with no tidal effect, the assumption of purely plug flow with no mixing may be reasonable. For this assumption, there is no effect on the upstream water of any waste discharged, whereas downstream water is affected as long as any of the waste is still present in the water. The rate of advective mass transport of a pollutant at any section of the river is given by $Q\ c$, where Q is the volume flow rate at the section and c is the concentration of the polluting substance expressed as mass per unit volume. In this case the resulting concentration of a conservative pollutant at any section of the river can be easily estimated knowing the amounts discharged at various upstream outfalls and the volume flow rate. For decaying substances the decay coefficient and the time of travel to the section from the outfalls are also required. [6]

Eddy Diffusion

Transport from high concentration to low concentration created by eddy diffusion is also responsible for the transport of pollutants in lakes, estuaries, and slow-moving streams. The term "eddy diffusion" is commonly used to cover the transport resulting from molecular and turbulent diffusion.

Fick's First Law for molecular diffusion states that the rate of mass transport is directly proportional to the average concentration gradient, or

$$\frac{\partial W}{\partial t} = -D_m \frac{\partial \bar{c}}{\partial x} \qquad (2\text{-}1)$$

in which W = diffusive transport and D_m is the molecular coefficient of diffusivity. The same form of equation is used to express eddy diffusion with D_m being replaced by E_x , the eddy diffusion coefficient.

Longitudinal Dispersion

The term "dispersion" is commonly used to cover the mixing resulting from pure molecular diffusion as well as that due to turbulence, stratification, and departures from one-dimensional flow resulting from shear flow. For shear flow in long channels the overall mixing resulting from the above phenomena is called "longitudinal dispersion." [7]

Dispersion processes have been investigated extensively in steady and open channel flows and theoretical values of the longitudinal dispersion coefficient proposed [7] based on certain parameters such as the "hydraulic radius" and "energy gradient." However, for most estuarine situations, the hydraulics are complex and these parameters cannot be defined. Hence it is common to rely on diffusion or dispersion coefficients determined by actual sampling of the estuary. Even for this purpose, a useful three-dimensional description of the dispersion process does not exist although progress is being made in this direction and two-dimensional models have now been established and tested. An approximation sufficient for the needs of this study can be obtained using a one-dimensional longitudinal model of estuarine dispersion in which the longitudinal dispersion coefficient E may vary with position and time.

Decaying Processes

The various substances that enter the water courses may be classified very broadly into degradable (nonconservative) and nondegradable (conservative) substances. Nondegradable pollutants (inorganic chemicals such as chlorides, pesticides, etc.) are not altered (at least rapidly) by the biochemical processes occurring in natural waters. Degradable pollutants such as BOD, forms of nitrogen, phosphorus, etc., are reduced relatively rapidly in form and sometimes in quantity by the action of the bacteria and other biota present in the receiving waters or by reaction with the receiving water constituents. If dissolved oxygen is available, aerobic degradation of carbon proceeds at a rate approximately proportional to the remaining concentration of unoxidized organic matter, giving a linear reaction rate. A very high concentration of degradable organic waste may consume all dissolved oxygen resulting in noxious anaerobic reactions which must be avoided in the receiving water.

The amount of oxygen used up by a degradable waste is called the Biochemical Oxygen Demand (BOD) for a particular time and water temperature. As the BOD is a measure of the concentration of biologically decomposable carbon present in polluted water it has become a common practice to use the term BOD in discussions of pollution load and concentration. Thus a biologically "hard" detergent is one which exerts a relatively low rate of BOD and is nearly conservative in natural waters whereas a biologically "soft" detergent has a relatively rapid BOD exertion and may be considered as a "nonconservative" pollutant even though both detergents could have the same oxygen requirements on a unit weight basis to be oxidized to the highest oxidation state.

DERIVATION OF THE DIFFUSION EQUATION

The one-dimensional form of the basic diffusion equation may be derived from mass continuity considerations of a constituent in an incremental volume of an estuary if it is assumed that the transport of constituent mass is strictly one-dimensional and in the longitudinal direction, through the cross section. Velocity and the dispersion coefficient are allowed to vary with x. At any section of the estuary, let

A = the average cross-sectional area
v = the average advective velocity
c = the average constituent concentration
E = the average longitudinal dispersion coefficient.

These averages denote the mean values taken over at least one but preferably several complete tidal cycles. The averages c , v , and E are taken over the cross-sectional area as well.

For purposes of the derivation it is assumed that:

1. The magnitude of the dispersion coefficient E is not influenced significantly by the nature of the constituent considered; i.e., it has the same value for all soluble or colloidal substances.

2. The dispersion coefficient E is an overall coefficient reflecting the turbulent mixing as well as dispersion caused by deviations from one-dimensional flow and density stratification.

3. The cross-sectional area $\bar{A}$ is constant from one tidal cycle to the next.

4. Reynold's axioms of turbulent flow [8] are valid.

In Figure 1 the mass transport of the constituent under study across the boundaries of an element of infinitesimal length dx is shown. As explained in the previous section, this involves two distinct processes, advection and eddy dispersion. The mass continuity of the constituent may be expressed as:

$$(\text{Input-Output})_{\text{advection}} + (\text{Input-Output})_{\text{dispersion}} + (\text{Sources-Sinks})$$

$$= (\text{changes in mass of the constituent contained in the element}).$$

The average mass transport rate through a section of cross-sectional area A by advection is given by Avc, and the rate due to eddy dispersion, by $-AE\,\partial c/\partial x$. Let S be the rate of discharge minus withdrawal of the constituent mass per unit length of the estuary at the same section. Then the mass continuity equation in the element of length dx during an infinitesimal interval dt is given by:

$$\left\{(Avc)dt - \left[Avc + \frac{\partial}{\partial x}(Avc)dx\right]dt\right\}$$

$$+ \left\{-\left(AE\frac{\partial c}{\partial x}\right)dt - \left[-AE\frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(-AE\frac{\partial c}{\partial x}\right)dx\right]dt\right\} \qquad (2\text{-}2)$$

$$+ Sdxdt = \frac{\partial}{\partial t}(Ac)\,dx\,dt \quad .$$

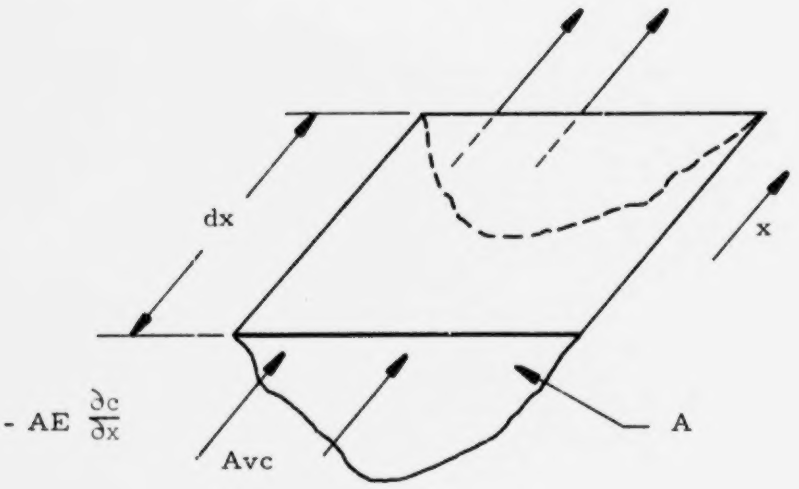

FIGURE I. ELEMENT OF INCREMENTAL VOLUME

By simplification:

$$-\frac{\partial}{\partial x}(Avc) + \frac{\partial}{\partial x}\left(AE\frac{\partial c}{\partial x}\right) + S = \frac{\partial}{\partial t}(Ac) \quad . \qquad (2\text{-}3)$$

In line with assumption 3, $\partial/\partial t\ (Ac) = A\ \partial c/\partial t$, and the one-dimensional nonsteady state diffusion equation becomes:*

$$\frac{\partial}{\partial x}\left(AE\frac{\partial c}{\partial x}\right) = \frac{\partial}{\partial x}(Avc) - S + A\frac{\partial c}{\partial t} \quad . \qquad (2\text{-}4)$$

Historically, Stommel [9] was one of the first to propose a steady state one-dimensional diffusion equation:

$$\frac{\partial}{\partial x}\left(AE\frac{\partial c}{\partial x}\right) = Q\frac{\partial c}{\partial x} \qquad (2\text{-}5)$$

where Q is the net advective flow at x , the other terms having the same interpretation as before.

Kent [10] generalized this equation for nonsteady conditions to obtain

$$\frac{\partial}{\partial x}\left(AE\frac{\partial c}{\partial x}\right) = Q\frac{\partial c}{\partial x} + A\frac{\partial c}{\partial t} \quad . \qquad (2\text{-}6)$$

Equation (2-6) which has been used in other investigations has the same general form as Equation (2-4).

Equation (2-4) is a linear first-order nonhomogeneous partial differential equation in E and is the basic nonsteady state diffusion equation relating waste discharges, which constitute the sources, to the resulting concentration levels. It expresses mathematically the physical and biochemical processes at work in an estuary (as long as the biological process can be expressed accurately as first-order rate of reaction). As noted earlier, if it is assumed that the effects of the dispersion process is negligible (a usual assumption [11] in the case of pollutional problems in rivers) this relation can be greatly simplified. But in dealing with estuarine pollution this simplification defeats the purpose and Equation (2-4) or some variation of it must be used.

---

*Though E is called the longitudinal dispersion coefficient, Equation (2-4) is equivalent in form to a diffusion equation with net advection.

Integrating Equation (2-4) seaward from the landward termination (origin) of the system gives

$$AE\frac{\partial c}{\partial x} = Avc - \int_{0}^{x} S\,dx + \int_{0}^{x} A\frac{\partial c}{\partial t}\,dx = Avc - T \qquad (2\text{-}7)$$

where T represents the average net rate of mass transport across a cross section at point x .

For a degradable substance, Equation (2-7) has the form

$$AE\frac{\partial c}{\partial x} = Avc - \int_{0}^{x} (S - k\,Ac)\,dx + \int_{0}^{x} A\frac{\partial c}{\partial t}\,dx \qquad (2\text{-}8)$$

in which k = first-order decay rate constant of the degradable substance in question, and S = net rate of constituent mass being created or destroyed per unit length of the element by external or internal sources or sinks. S now accounts for all discharges and withdrawals but excludes the decaying process of the substance by biochemical reaction which is now included in a separate term.

Inputs to a natural estuary are rarely steady, even if the tidal averages are considered. In fact, the concentration profiles of most substances usually never attain a steady state condition in natural estuaries because hydrologic factors usually undergo seasonal alteration before the constituent can attain a steady distribution. However, possibly due to the high rate of decay, the concentration profile for degradable substances may attain a steady state in a relatively few days if the sources of the constituents are steady. Hence, as a preliminary attack on the problem, steady conditions based on average values A , E , v , and c over tidal cycles is herein considered. With steady state assumptions the diffusion equation for a nonconservative substance has the form:

$$AE\frac{dc}{dx} = Avc - \int_{0}^{x} (S - k\,Ac)dx \quad . \qquad (2\text{-}9)$$

For a conservative substance, the form of the equation is:

$$AE\frac{dc}{dx} = Avc - \int_{0}^{x} S\,dx \quad . \qquad (2\text{-}10)$$

The mixing and the resulting concentration profile for each constituent relevant to water quality can be predicted with the aid of the above equations if the required hydrological data and parameters are known. In all cases the solutions may be approximated by using one of several available numerical methods. It is almost impossible to obtain values of A , E , and v as continuous functions of x or x and t , without making some approximations. The usual practice is to measure A and v at discrete points along the length of the estuary. One of the main difficulties is to obtain values of E , since no satisfactory theoretical method of obtaining E *a priori* exists today. However, Equation (2-7) has been successfully applied to compute values of E at discrete points along the length of the estuary from measured concentration profiles of chloride and silica obtained by actual sampling. This method was used during an extensive investigation in the San Francisco Bay conducted by Glenne, Selleck, and Pearson [12]. They applied the method to estimate dispersion coefficients at discrete sections of the Bay system, which along with other hydrological data, were then used to predict concentration profiles under steady and non-steady conditions. These profiles compared favorably with the concentration values obtained by field observations.

Thus a method of predicting the concentrations (the output or the effects) of chemical components resulting from the discharge of pollutants (given input or causes) is available, through the use of the diffusion equation. In the section entitled OPTIMIZATION PROBLEM, further consideration is given to how one should control the discharge of pollutants in an optimal fashion to have the desired levels of concentration at various sections of the estuary. For the present discussion, it is assumed that there are no sinks for the constituent in the estuary; i.e., S consists of sources only. The representation of sinks requires only minor modifications in the models if Q_{Li} , the quantity of water withdrawn from section i of the estuary, is known.*

HYDROLOGY OF THE ESTUARY

If steady state conditions are assumed Equations (2-9) and (2-10) represent the dispersion and advection processes at a section of the estuary for decaying and conservative substances, respectively. The parameters A , E , and v are rarely constant along the length of the estuary and the dispersion process will be determined by the nature of these functions. Simple algebraic forms for these functions, are herein assumed so that analytical results (Chapter IV) may be obtained for some representative situations. Equations (2-9) and (2-10) may be rewritten as

$$\frac{dc}{dx} = ac - b \int_0^x (S - k\,Ac)dx \qquad (2\text{-}11)^{**}$$

and

$$\frac{dc}{dx} = ac - b \int_0^x S\,dx \qquad (2\text{-}12)^{**}$$

where

$$a = \frac{v}{E} \text{ , } b = \frac{1}{AE} \text{ and } \frac{a}{b} = Av = Q \text{ .}$$

Q represents the volume flow at a section of the estuary and following O'Connor [11], who studies streams for variations of volume of flow and cross-sectional area, the three following cases are considered:

Case A: $Q(x)$ is independent of x and equal to Q_o .

Case B: $Q(x)$ is a linear function of x , usually increasing downstream due to increases in drainage and ground water flow and $Q(x) = Q_o\,(1 + qx)$ where Q_o is the flow at the origin and q is a constant. This case applies to a large number of streams.

Case C: $Q(x)$ is an exponential function, usually increasing with x and given by $Q(x) = Q_o\,e^{gt}$ where g is a constant for an estuary. This assumption sometimes holds for an estuary near the ocean.

Similary for each of the above cases the same three functions are chosen to represent the changes in cross-sectional area [11]. As $A(x)v(x) = Q(x)$, the velocity $v(x)$ is now determined at any section. For simplicity we assume E to be constant along the estuary, though a study in the northern section of San Francisco Bay [12] showed that E varies directly with $v^{3/4}$. Table I shows the values of $a(x)$ and $b(x)$ for the various forms of $Q(x)$ and $A(x)$ described above.

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*See the following footnote and AN ALTERNATIVE DISCRETE STEADY STATE FORMULATION in Chapter V.

**If there are sinks present in the estuary and $Q_L(x)$, the rate of withdrawal per unit length at section x , is known then S is replaced by $S - Q_L(x)\,c(x)$ in Equations (2-11) and (2-12).

TABLE I

VALUES OF $a(x)$ AND $b(x)$ UNDER SIMPLIFIED ASSUMPTIONS

			Cross-Sectional Area		
	Volume Flow $Q(x)$		1. Constant $A(x) = A_o$	2. Linear $A(x) = A_o(1 + k_1 x)$	3. Exponential $A(x) = A_o e^{k_2 x}$
Case A	Constant $Q(x) = Q_o$	$a(x)$	a_o	$a_o(1 + k_1 x)^{-1}$	$a_o e^{-k_2 x}$
		$b(x)$	b_o	$b_o(1 + k_1 x)^{-1}$	$b_o e^{-k_2 x}$
Case B	Linear $Q(x) = Q_o(1 + qx)$	$a(x)$	$a_o(1 + qx)$	$a_o(1 + qx)(1 + k_1 x)^{-1}$	$a_o(1 + qx) e^{-k_2 x}$
		$b(x)$	b_o	$b_o(1 + k_1 x)^{-1}$	$b_o e^{-k_2 x}$
Case C	Exponential $Q(x) = Q_o e^{\varepsilon x}$	$a(x)$	$a_o e^{\varepsilon x}$	$a_o e^{\varepsilon x}(1 + k_1 x)^{-1}$	$a_o e^{(\varepsilon - k_2)x}$
		$b(x)$	b_o	$b_o(1 + k_1 x)^{-1}$	$b_o e^{-k_2 x}$

NOTE:

$a_o = \frac{v_o}{E} \quad b_o = \frac{1}{A_o E}$

The subscript o refers to the value of the corresponding function at the origin.

In a tidal estuary, the tidal volume flow decreases upstream. If $Q(x)$ represents an average downstream volume flow, due to excessive evaporation and other sinks in the estuary, $Q(x)$ may even decrease downstream. In Case B, q may be taken as negative; in Case C, either g is negative or $Q(x) - Q_o \cdot (1 - e^{gt})$ may represent this situation. This decrease in $Q(x)$ was observed in Suisun Bay and San Pablo Bay when computations were done using data presented in [12].

BOUNDARY CONDITIONS

As in any other physical system, proper boundary conditions must be specified as they affect and constrain the behavior of the system. In the one-dimensional diffusion model, one boundary condition is needed at each end of the estuary. In a natural estuary, it is difficult to evaluate the limits of the regime because it tends to blend gradually into a river system at the landward end and an ocean regime at the seaward end. Hence, some judgment is required to select limits which will allow reasonable simulation of the events occurring in the actual estuary.

In the ocean end of the estuary, due to the almost infinite amount of dilution and dispersion experienced by the discharge of the estuary, the concentration of most of the water constituents reach a stationary value near the oceanic level of each constituent and this may be taken as a boundary condition. Though the exact location of this boundary $(x = L)$ is not easily determined, the concentration of a pollutant at such a boundary may be considered independent of the discharge plans, especially for degradable substances like BOD. However, as the pollution load is increased too much in the estuary, this boundary will tend to move farther out into the ocean.

Another approach is to take the concentration $c(\infty) = 0$. However, Equation (2-13) will be assumed here to hold for all discharge plans.

$$C(L) = \text{Oceanic Level (0 for many pollutants)} . \qquad (2\text{-}13)$$

In the landward end $(x = 0)$, the boundary condition may be expressed by Equation (2-14) which is essentially the same as Equation (2-7).

$$T_o = (Avc)_{x=o} - \left(AE \frac{dc}{dx}\right)_{x=o} . \qquad (2\text{-}14)$$

To represent the overall net transport rate of constituent mass into the region at the boundary $x = 0$, the magnitude of T_o may be measured in the field or estimated from other considerations. The following are a few special cases [12]:

1. Insignificant external sources and sinks of the constituent landward of the boundary: $T_o = 0$.
2. Insignificant volume of water landward of the boundary: T_o is the net total of all external sources and sinks landward of the boundary.
3. Significant volume of water landward of the boundary:
    a. Conservative constituent: Same as 2 above.
    b. Nonconservative constituent: T_o is the actual amount of the constituent crossing into the boundary at $x = 0$, obtained by measurement or computation.

The pollution problem in the river system feeding an estuary may be much more critical than in the estuary itself. It is usually advisable to include the river system to a significant upstream length into the reach of the diffusion model. This is especially important in the river systems experiencing substantial longitudinal mixing due to tidal currents and having low advective velocity. A large number of models of water pollution control [6, 11, 13] neglect logitudinal dispersion and use a simplified mass continuity model. These models are inaccurate to the extent that E may have a very high value near the ocean. However, at a significant distance from the ocean upstream, where E is low and v is high, a simplified boundary condition may be used.

If $\left(AE \frac{dc}{dx}\right)_{x=o} \ll (Avc)_{x=o}$, then $T_o \simeq (Avc)_{x=o}$. Hence, knowing T_o as before, we can assume a boundary condition

$$C(0) = \frac{T_o}{A(0)v(0)} \quad . \qquad (2\text{-}15)$$

Assuming Equation (2-14) to represent the boundary condition at the landward end of the estuary we can modify Equation (2-12) to include the T_o term.

$$\frac{dc(x)}{dx} = a(x)c(x) - b(x)\int_o^x S(x)\,dx - T_o\,b(x) \quad . \qquad (2\text{-}16)$$

Equation (2-11) will also be similarly modified.

OPTIMIZATION PROBLEM

One of the basic objectives of resource management is the optimum utilization of the resources. Water quality may be considered as a natural resource useful for waste disposal purposes. The fact that this resource is scarce and deserves optimal allocation need not be overemphasized. In this section and also in Chapter VI and VII optimization models are presented which involve an estuarine water basin used for effluent disposal by various public (city or municipal) and private dischargers.

In these models, it is assumed that the quality of water in the basin is characterized by the resulting concentration of certain chemical* characteristics or components such as biochemical oxygen demand, chlorides, nitrogen, phenol, boron, phosphates, etc., which are discharged into the basin. An optimal quality control program is then sought for the entire basin. This can be done with various levels of sophistication in four ways:

1. For a given amount of waste material to be discharged, minimize the adverse effects of high concentration using the hydrological and self-purifying properties of the water in an optimal fashion.
2. Specify acceptable quality standards and obtain a plan which minimizes the total pollution abatement (or waste treatment) cost while maintaining concentration of each of the polluting components at a value less than or equal to the prescribed quality standard.
3. Express social damage and/or opportunity cost of pollution in terms of the concentration of the polluting components and minimize the sum of the social damage and abatement costs.
4. A synthesis of the last two approaches may be used.

The relative merits of these approaches are discussed and are illustrated in the models described below.

These models are based on the following five main assumptions in addition to those stated in the Derivation of the Diffusion Equation.

---

*Thermal and radiation pollution may become significant in certain basins.

A1. The dispersion characteristics of the body of water being studied may be approximated by a one-dimensional dispersion model

A2. The conservative constituents discharged into the water do not react appreciably with each other to affect their concentrations. For nonconservative substances, the reaction rate is always linear having the form $r_A = -k(c_A - k_1)$ where k and k_1 are constants and $k_1 \geq 0$.

A3. Steady state conditions have been assumed averaging over a tidal cycle.

A4. The flow of waste discharges do not appreciably influence the net advection in the system.

Models A, B, and C have been formulated for conservative constituents. For converting them to decaying substances, Equation (2-9) modified for boundary conditions will replace Equation (2-16) in Models A and B and Equation (2-25) in Model C.

Model A

The basic idea of this model is the optimal allocation of water quality throughout an estuary by controlling the discharge pattern. Water quality problems are usually characterized by very high concentrations of pollutants at certain areas of the water body, the rest of the water being at a much lower state of pollution. This is due to an uneven and nonoptimal discharge pattern along the estuary. Since the maximum concentration of a constituent is the critical factor (minimum in case of dissolved oxygen) which often determines the damage costs, and the object is to keep it as low as possible, the following problems may be posed.

Problem A. Given the total quantity of a pollutant to be discharged into the estuarine water, determine the locations of outfalls and quantities to be discharged at these locations, so that the maximum concentration of the pollutant over the estuarine basin is minimized.

In case the locations are fixed, only the quantities to be discharged at these locations serve as the control variables.

A one-dimensional estuary is shown in Figure 2 with the notations of the model explained.

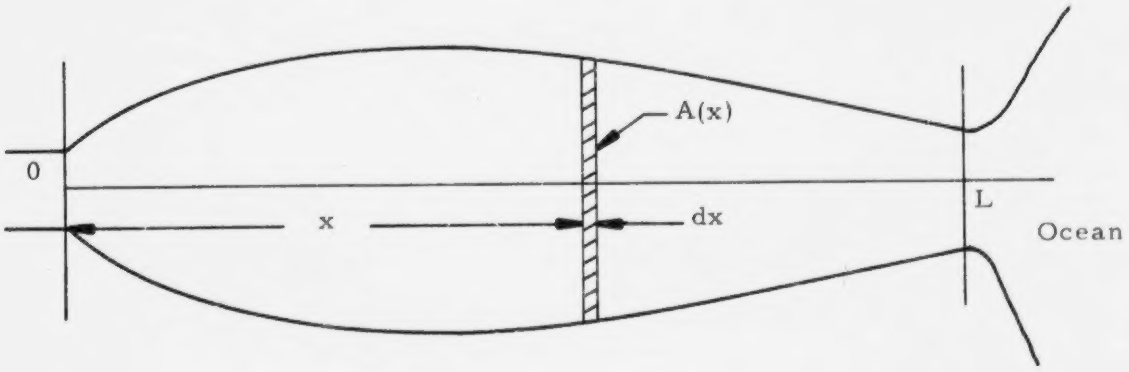

FIGURE 2. SKETCH OF AN ESTUARY

For this purpose Equation (2-16) may be rewritten

$$\frac{dc_s(x)}{dx} = a(x)c_s(x) - b(x) \int_0^x S(x)\,dx - T_0\,b(x) \qquad (2\text{-}16)$$

$$0 \leqq x \leqq L\ ,\ c_s(L) = c_L \quad \text{(given constant).}$$

$S(x)$ is a measurable function which represents the rate of discharge per unit length per unit time at section x . Integrating $S(x)$ with respect to x , the cumulative discharge function is as shown in Figure 3.

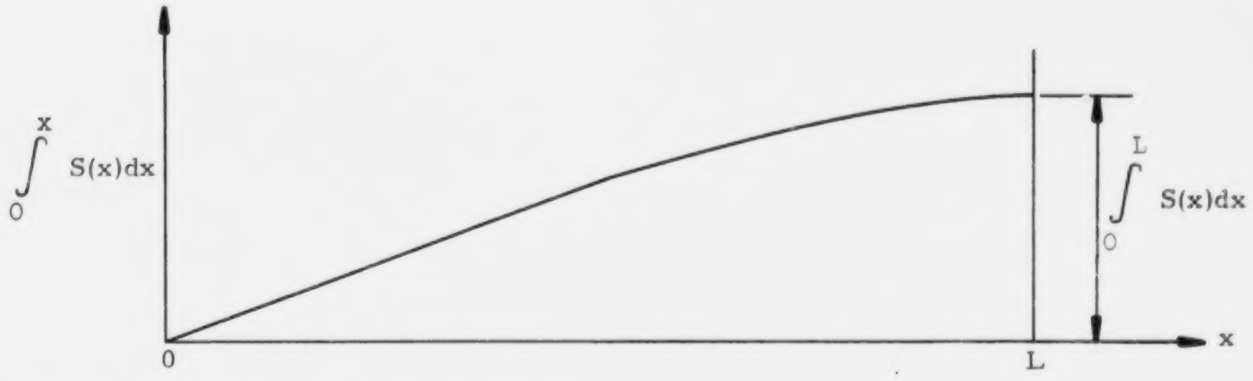

FIGURE 3. CUMULATIVE DISCHARGE FUNCTION

Given the total amount of discharge $\overline{S}$ over the whole stretch of the estuary, $S(x)$ must satisfy the condition

$$\int_0^L S(x)dx = \overline{S}\ ,\ 0 \leqq L_s(x) \leqq S(x) \leqq U_s(x)\ \forall\ x \in [0\ ,\ L] \qquad (2\text{-}17)$$

where $U_b(x)$ and $L_s(x)$ are the upper and lower bounds on the discharge rate from physical considerations, basically to avoid very high local concentration near the outfall. Let S^* be the set of all S satisfying Equation (2-17).

$$S^* = \left\{ S\ :\ L_s(x) \leqq S(x) \leqq U_s(x)\ \forall\ x \in [0\ ,\ L] \ \text{ and } \int_0^L S(x)dx = \overline{S} \right\} .$$

Problem A, can now be stated precisely: Given $S \in S^*$, analytical or numerical methods may be used to solve Equation (2-16) if the hydrological character of the estuary and the diffusion coefficients are known. A profile of concentration ($c(x)$) of the constituent along x-axis (Figure 4) is obtained.

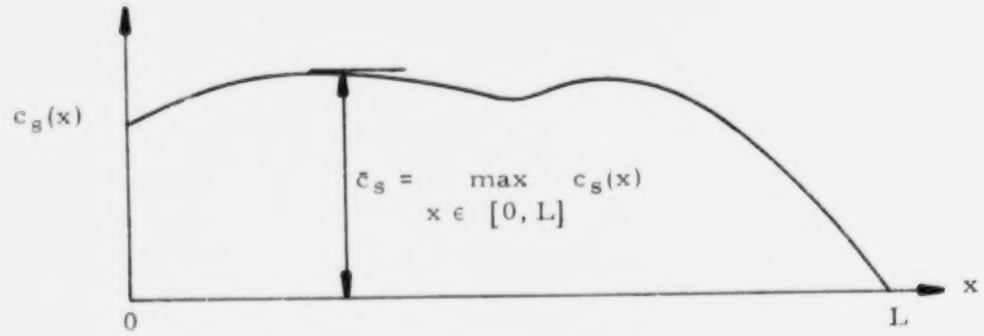

FIGURE 4. CONCENTRATION PROFILE IN AN ESTUARY

Let $\bar{c}_s = \max_{x\epsilon[0,L]} c_s(x)$ where $c_s(x)$ satisfies Equation (2-16) for some $S \epsilon S^*$ and $c_s(L) = c_L$ (given) and

$$c^* = \min_{S\epsilon S^*} \left[\bar{c}_s \right] = \min_{S\epsilon S^*} \left[\max_{x\epsilon[0,L]} c_s(x) \right] \quad . \tag{2-18}$$

Now Problem A may be stated as:

Find c^* and $S \epsilon S^*$ satisfying equations (2-16), (2-17), and (2-18).

This mathematical programming problem does not immediately seem to be amenable to a simple computational approach due to the presence of the differential equation. Problem A could be formulated as a linear optimal control problem with a state variable constraint. This approach is useful if $E(x)$, $A(x)$, and $v(x)$ could be expressed as simple continuous functions so that closed form solutions may be obtained. But this is often difficult with data obtained from sampling studies. However, the continuity of the physical process may be approximated by discretization. As shown in Chapter V, under these assumptions, Problem A can be formulated as a Linear Programming Problem. The similarity of the Minimax problem to the Linear Programming formulation of a Two-Person zero-sum game is noticeable which might have been suspected from Equation (2-18).

Model B

Here it is assumed that the objective in designing an efficient Water Quality Management System is to maintain a quality standard expressed in maximum allowable concentrations (and arrived at from health, wildlife, and other considerations by a regional or governmental authoritative body) at minimum cost of waste treatment. It may also be desired to study various alternative quality objectives and the corresponding costs. To obtain this objective, Problem B is proposed.

Problem B. Given maximum allowable concentrations $U_c(x)$ of various polluting constituents at different sections of an estuary, obtain a plan which maximizes the total amount discharged for each constituent. This will minimize the total amount of the pollutants to be removed from the raw effluents before discharging into the estuarine water, presumably minimizing treatment cost.

Expressed mathematically, Problem B reads

$$\text{Find } D = \max \int_0^L S(x)dx \ , \ S \epsilon S^{**} \tag{2-19}$$

and obtain the corresponding optimal discharge pattern $\tilde{S}(x)$. S^{**} is the set of feasible discharge patterns S satisfying equations (2-16), (2-20), and (2-21) and any other arbitrary constraint that might be imposed;

$$0 \leqq L_s(x) \leqq S(x) \leqq U_s(x) \ , \ x \in [0 \ , \ L] \tag{2-20}$$

and

$$0 \leqq c_s(x) \leqq U_c(x) \ , \ x \in [0 \ , \ L] \tag{2-21}$$

where $c_s(x)$ is evaluated from Equation (2-16) from some $S(x)$ satisfying Equation (2-20) and $c_s(L) = c_L$.

$$\frac{dc_s(x)}{dx} = a(x)c_s(x) - b(x)\int_0^x S(y)dy - T_o\, b(x) \ , \ x \in [0 \ , \ L] \ . \tag{2-16}$$

Problem B is also transformed into a linear optimal control problem with a state variable constraint in Chapter IV. As shown in Chapter V, if Equation (2-16) is expressed as a set of difference equations, Problem B becomes a Linear Program. A duality relation, different from the conventional duality concept of linear programming, exists between Problems A and B and is discussed in Chapter III.

Model B as Stage 1 and the Waste Treatment Model of Chapter VI as Stage II, form the basic model of optimal water quality management in this report and their synthesis into a single model is discussed in Chapter VII. Various alternative quality objectives and their corresponding costs may be studied by using different sets of values for $U_c(x)$.

Model C

There are various social costs associated with the degradation of water quality. These may be due to the damage to the fish and wildlife, cost of pretreatment required at various intakes and/or damage to the machinery and equipment used, effects on aesthetic and recreational aspects of the water body, and the gradual decay of the water resources.

These social costs were not explicitly taken into account in Model B. A quality standard expressed as maximum allowable concentration levels for various polluting substances effectively gives a step function for social cost, the cost being zero for allowable concentrations, and infinite if the limits are crossed. If more detailed information on the social costs are available, a more general social cost function may be used.

Assume water quality is characterized by M polluting components and $c(x)$ is the M-vector of concentration levels of the M components at the section x of the estuary. Similarly, let $S(x)$ be the M-vector of discharge rates of the components per unit length at a distance x in the estuary. Let $h : R^M \rightarrow R$, and $h(c(x))$ be the function representing social cost rate of pollution per unit length of the estuary at section x due to a level of water quality expressed by $c(x)$.

Given the total load of polluting substances generated in the estuarine basin, a saving can be effected whenever discharge of an amount of the substance in the estuary is allowed; otherwise it is necessary to treat this amount at added cost. Let $\ell : R^M \rightarrow R$, and $\ell(S(x))$ be the function representing the savings rate per unit length of the estuary at section x corresponding to a discharge rate vector $S(x)$.

Assuming that the objective is to minimize the social cost of pollution, less the savings accrued by discharging over the entire estuarine basin, the concentration levels can still be limited by providing upper bounds $U_c(x)$ or by assuming that the cost $h(c(x))$ becomes infinite whenever $c(x)$ is outside the feasible region defined by the upper bounds $c^m(x) \leqq U_c^m(x)$, $m = 1, 2, \ldots, M$, $x \in [0 \ , \ L]$. To obtain this objective Problem C is proposed.

Problem C.

$$\text{Minimize } TC = \int_0^L h(c(x))dx - \int_0^L \ell(S(x))dx \ , \ S(x) \in S \qquad (2\text{-}22)$$

in which S is the set of feasible discharge patterns satisfying Equation (2-23) and such that $c^m(x)$ evaluated from Equation (2-25) satisfies Equation (2-24).

$$\left.\begin{array}{r} 0 \leqq L_S^m(x) \leqq S^m(x) \leqq U_S^m(x) \\ 0 \leqq c^m(x) \leqq U_C^m(x) \end{array}\right\} \begin{array}{l} m = 1, 2, \ldots, M \qquad (2\text{-}23) \\ x \in [0 \ , L] \ . \qquad (2\text{-}24) \end{array}$$

$$\frac{dc^m(x)}{dx} = a(x)c^m(x) - b(x)\int_0^x S^m(x)dx - T_0^m b(x) \ , \quad m = 1, 2, \ldots, M \qquad (2\text{-}25)$$

$$x \in [0 \ , L] \ .$$

Unsteady State Models

In Assumption 3 (page 14), steady state conditions averaged over a complete tidal cycle were assumed for area, velocity, diffusion coefficient, mass flow, and discharge rate. These assumptions may be valid for a period of a few weeks but seasonal changes take place in all estuaries. The flow of water may be reduced during summer months, aggravating the quality problem. The waste generation rates may also be subject to seasonal variations as, for example, in the canning industry. The parameters of the diffusion equation also may change. Thus the need for an unsteady state model is very realistic.

The models previously discussed in this chapter may be converted to unsteady state models by replacing Equations (2-16) or (2-25) by (2-4) where the concentration $c(x,t)$ and discharge rate $S(x,t)$ are expressed as a function of two parameters, space and time. When formulated as continuous diffusion models, they give rise to distributed parameter control problems which are highly involved. However, when discretized they become linear programs as illustrated in Chapter V.

III. A DUALITY THEORY FOR A CONTINUOUS MATHEMATICAL PROGRAMMING PROBLEM

INTRODUCTION

The optimal control Problems A and B in Chapter II have been formulated in such a way that in Problem A, given the total amount of the constituent discharged, the maximum concentration is minimized; whereas in Problem B, exactly the opposite case is solved by maximizing the total amount discharged, given the maximum allowable concentration of the constituent. From the physical nature of the diffusion model, one would suspect that there exists some kind of duality relation between these two problems. A special kind of a strong duality relation between these two problems, different from the conventional duality concept in mathematical programming [14], can be shown to exist.

A DUALITY THEOREM

Problem A is described by equations (2-16), (2-17) and (2-18) in Chapter II and Problem B by equations (2-16), (2-19), (2-20) and (2-21). To obtain a meaningful duality relation, it is assumed that

$$\left.\begin{array}{c} U_s(x) \equiv U_s \\ L_s(x) \equiv L_s \\ \text{and} \\ U_c(x) \equiv U_c \end{array}\right\} \quad 0 \leqq x \leqq L \ .$$

The duality theorems of this chapter basically state that if both Problems A and B are solved successively with $U_c = c^*$, D will equal $\overline{S}$ or vice versa. In subsequent paragraphs these are expressed as Theorems (3-2) and (3-3). However, it is first necessary to establish what is herein called Theorem (3-1).

Theorem (3-1)

For Problem B, the maximum discharge quantity D is a strictly increasing function of the maximum allowable concentration level U_c in the region $0 \leqq L_s\, L \leqq D < U_s\, L$.

Proof

Suppose, for a given value of U_c , Problem B is solved to obtain an optimum solution S^*, c_s^*, and $D^* = \max\limits_{S \epsilon S^{**}} \int_0^L S(x)\, dx$ with $0 \leqq L_s\, L \leqq D^* < U_s\, L$. As $D^* < U_s\, L$, and $S^*(x) \leqq U_s \ \forall\ x \ \epsilon\ [0\ ,\ L]$, for some $\Delta > 0$, there exists a set $E \ \epsilon\ [0\ ,\ L]$ of positive measure ϵ such that $S^*(x) < U_s - \Delta$ on E.

It can be shown that $c_s^*(x) = U_c$ for some point x in $[0\ ,\ L]$. If not, then $c_s^*(x) < U_c \ \forall\ x \ \epsilon\ [0\ ,\ L]$ and in fact from the continuity of c_s^* , $c_s^*(x) < U_c - \delta$, $\delta > 0 \ \forall\ x \ \epsilon\ [0\ ,\ L]$.

$$\text{Defining } \widetilde{S} = \begin{cases} S^* \text{ on } [0\ ,\ L] - E \\ S^* + \Delta_1 \text{ on } E \end{cases}$$

for some as yet unspecified $0 < \Delta_1 \leqq \Delta$, and letting $\widetilde{c}_s$ and $\widetilde{D}$ be the new solution, the function $c_s(x)$ as the solution of

$$\frac{dc_s}{dx} = a\ c_s - b \int_0^x S(y)\ dy - b\ T_o\ ,\ c_s(L) = c_L$$ (given constant) depends continuously on $b \int_0^x S(y)\ dy$ and hence for Δ_1 sufficiently small, $\widetilde{c}_s(x)$ remains less than $U_c\ \forall\ x \in [0\ ,\ L]$. Hence the new solution is feasible. But $\widetilde{D} - D^* = \int_0^L \widetilde{S}(y)\ dy - \int_0^L S^*(y)\ dy = \Delta_1\ \epsilon > 0$ which contradicts that D^* represents an optimal solution.

Now suppose that $c_s^*(x) = U_c$ in the optimal solution and the problem is changed by increasing U_c to $U_c + \epsilon$, $\epsilon > 0$, so that $\forall\ x$, $c_s^*(x) < U_c + \epsilon$. Clearly $c_s^*(x)$ could not be the optimal solution to the modified problem and as in the proof given above, $S^*(x)$ can be increased to $\widetilde{S}(x) = S^*(x) + \Delta_1$ on E , thus obtaining $\widetilde{D} = \int_0^L \widetilde{S}(y)\ dy > D^*$. Hence the new optimal value $D(\epsilon) \geqq \widetilde{D} > D^*$. Essentially what is proved is that D is a strictly increasing function of U_c . Note that if $D = U_s\ L$, no further increase of U_c will change D from its maximum value.

Q.E.D.

Theorem (3-2)

The first duality Theorem (3-2) is the converse of Theorem (3-4), which needs Lemma (3-3) for its proof. Lemma (3-3) in turn depends on (3-1) and (3-2) for its proof.

Let D^* $(D^* < U_s\ L)$ be the value of the optimum solution for Problem B with $U_c(x) \equiv U_c$ for $0 \leqq x \leqq L$. If Problem A is solved with $\overline{S} = D^*$, the value of the optimal solution c^* will equal U_c .

Proof

Let $c_{sB}(x)$ and $S_B(x)$, $0 \leqq x \leqq L$ represent an optimal solution of Problem B, and D^* its value. $c_{sB}(x)$ and $S_B(x)$ satisfy Problem A with $\overline{S} = D^*$ from the definition of Problems A and B. As c^* is minimum for Problem A with $\overline{S} = D^*$, we must have $c^* \leqq U_c$.

Assuming $c^* < U_c$, Problem B may be again solved with $U_c(x) = c^*$ for $0 \leqq x \leqq L$. Let D^{**} be the new maximum value of the objective function. To be optimal for the modified Problem B, $D^{**} \geqq D^*$. Otherwise, the optimal solution of Problem A (with $\overline{S} = D^*$) given by, say, $c_{sA}(x)$ and $S_A(x)$, $0 \leqq x \leqq L$, which is also feasible for Problem B, will give a higher value of $D = \int_0^L S(y)\ dy$.

But from Theorem (3-1), $D^{**} < D^*$, if $c^* < U_c$, this is a contradiction. Hence $c^* = U_c$.

As a consequence, $c_{SB}(x)$ and $S_B(x)$, for $0 \leqq x \leqq L$, also constitute an optimal solution for Problem A with $\overline{S} = D^*$.

Lemma (3-3)

For Problem A, the minimum value of maximum concentration c^* is a strictly increasing function of the total amount discharged $\overline{S}$ in the range $0 \leqq \overline{S} < L\, U_s$.

Proof

Let D^1 and D^2 be the optimal values of D for Problem B with $U_c(x) = U_c^1$ and U_c^2 , respectively, where $U_c^2 > U_c^1$. Then from Lemma (3-1) $D^2 > D^1$. Applying Theorem (3-2), if Problem A is solved with $\overline{S} = D^1$, the optimal solution $c^{1*} = U_c^1$; again if Problem A is solved with $\overline{S} = D^2$, the optimal solution $c^{2*} = U_c^2$. Here $U_c^2 > U_c^1$ appears as $c^{2*} > c^{1*}$. But $D^2 > D^1$.

Hence, it is proved that c^* is a strictly increasing function of $\overline{S}$ in the range $0 \leqq L\, L_s \leqq \overline{S} < L\, U_s$. (This condition is necessary in order to apply Theorem (3-2).)

Theorem (3-4)

Let c^* be the value of the optimal solution for Problem A. If Problem B is solved with $U_c = c^*$, then the value of the optimal solution D^* will equal $\overline{S}$ of Problem A.

Proof

Let $c_{SA}(x)$ and $S_A(x)$, $0 \leqq x \leqq L$, represent an optimum solution of Problem A and c^* its value.

$c_{SA}(x)$ and $S_A(x)$, $0 \leqq x \leqq L$, satisfy Problem B with $U_c = c^*$, from the definition of Problems A and B. As D^* is maximum for Problem B with $U_c = c^*$,

$$D^* \geqq \overline{S} = \int_0^L S_A(y)\, dy \ .$$

Assuming $D^* > \overline{S}$, Problem A may be solved again with $\int_0^L S(y)\, dy = D^*$. Let c^{**} be the new minimum value of the objective function. To be optimal for the modified Problem A, $c^{**} \leqq c^*$ must hold. Otherwise, the optimal solution of Problem B (with $U_c = c^*$) given by, say, $c_{SB}(x)$ and $S_B(x)$, $0 \leqq x \leqq L$, which is also feasible for Problem A, will give a lower value of the objective function.

But from Lemma (3-2), $c^{**} > c^*$ if $D^* > \overline{S}$ must be a contradiction. Hence $D^* = \overline{S}$. As a consequence, it is evident that $c_{SA}(x)$ and $S_A(x)$ for $0 \leqq x \leqq L$ also constitute an optimal solution for Problem B with $U_c = c^*$. Q.E.D.

The most interesting aspect of the duality (3-3) between the two continuous mathematical programming (or optimal control) problems is that when one of them is solved the solution also solves the other problem for a particular value of one of its parameters.

One of the problems is a maximizing problem and the other a minimizing problem, and at optimality certain equality relations hold between them. Herein lies a difference from the duality principle of linear programming. At optimality, equality holds between the objective function of one problem and the right-hand side value of a constraint of the other and is conditional on a similar equality in the opposite direction. In this case both the problems share the same differential equations and both share the same variables too.

Perhaps this duality principle could be generalized to a wider class of similarly posed optimal control problems representing physical systems. This is useful as often one of the two problems may be easier to solve and valuable insight regarding the solution of the other problem could be obtained.

IV. LINEAR OPTIMAL CONTROL THEORY AND THE CONTINUOUS DISPERSION MODEL

INTRODUCTION

During the last two decades, Optimal Control Theory and the related Maximum Principle [15] are increasingly used in the design, operation, and control of engineering and physical systems and they have come far away from the mathematical obscurity enjoyed by Calculus of Variations, a closely related field. So it is no wonder that optimal control theory will prove useful in the optimization of the physical process of dispersion of pollutants in an estuary. This process has been described in Chapter II by a partial differential equation in the unsteady state case and an ordinary differential equation with steady state assumptions. This chapter deals with the general solutions of steady state dispersion models, conceived in Chapter II, reformulated as linear optimal control problems with state variable constraints. The unsteady state case gives rise to distributed parameter control problems which are usually more involved.

Before proceeding with the solutions of problems B and C of Chapter II, it is first necessary to derive results from four specific problem situations:

1. Linear optimal control problem

2. Minimum principle for linear optimal control problem

3. Transversality conditions

4. Linear optimal control problem with State variable constraints.

LINEAR OPTIMAL CONTROL PROBLEM

In its standard form a linear system is specified completely by the values of its "state" vector, and its transition in "state space" with time is described by a linear differential vector equation involving the "state" vector and a "control" vector (to be chosen from a specified control set). The linear optimal control problem involves finding an admissible control vector and the corresponding trajectory described by the state vector which minimizes a linear functional of the state and control vectors while the system is transferred from an initial state to a terminal target state.

Mathematically the problem is to:

$$\begin{aligned}
&\text{minimize} \quad x_0(T) \\
&\text{subject to} \quad x(t_0) = x^0 \; ; \quad x^0 \in E^{n+1} \\
&\qquad x_i(T) = x_i^T \; ; \quad i = 1, 2, \ldots, n \; ; \quad \left(x_1^T , \ldots, x_n^T\right) \in E^n \qquad (4\text{-}1) \\
&\qquad \frac{dx(t)}{dt} = A(t)x(t) + B(t)u(t) \; ; \quad u \in \Omega \, , \quad t_0 \leq t \leq T \, ,
\end{aligned}$$

where $A(t)$ and $B(t)$ are $(n + 1) \times (n + 1)$ and $(n + 1) \times r$ matrices, respectively. Then $x(t)$ is an $(n + 1)$-dimensional state vector and $u(t)$ is an r-dimensional control vector. E^n is the n-dimensional euclidean space. $dx(t)/dt$ is an $(n + 1)$-dimensional vector of derivatives $dx_i(t)/dt$. $i = 0, 1, \ldots, n$ for $t_0 \leq t \leq T$.

The following assumptions are made:

A1. The elements $a_{ij}(t)$ of $A(t)$ and $b_{ij}(t)$ of $B(t)$ are continuous on $[t_o, T]$.

A2. The control function $u : [t_o, T] \rightarrow R$ belongs to the set Ω defined by: $\Omega = \{u : u \text{ is measurable and } u(t) \in P(t) \text{ where } P(t) \subset E^r \ \forall\, t \in [t_o, T]\}$.

A3. $P(t)$ of (A2) is convex and compact for all t , $t_o \leqq t \leqq T$, and $P(t)$ hausdorff continuous in t .

Consider first the case where the control vector is identically zero; that is, for all $t \in [t_o, T]$.

$$\frac{dx(t)}{dt} = A(t)x(t) . \tag{4-2}$$

For the linear system Equation (4-2), where the elements $a_{ij}(t)$ of $A(t)$ are continuous on $[t_o, T]$, there is one and only one solution $x(t;\, x^o,\, t_o)$ of (4-2) on $[t_o, T]$ passing through the state x^o at time t_o [16]. The expression for this solution is given in the following Theorem (4.3).

Theorem (4.3)

Let $A(t)$ be the $(n + 1) \times (n + 1)$ matrix whose elements are continuous functions on $[t_o, T]$. Let $\Phi(t, t_o)$ be the $(n + 1) \times (n + 1)$ matrix which is the solution of the equations:

$$\frac{d}{dt}\,\Phi(t,\, t_o) = A(t)\Phi(t,\, t_o) \ ; \quad \Phi(t_o,\, t_o) = I \text{ , the identity matrix.} \tag{4-4}$$

Then the solution to the equation

$$\frac{dx(t)}{dt} = A(t)x(t) \ ; \quad x(t_o) = x^o , \tag{4-2}$$

denoted by $x(t;\, x^o,\, t_o)$ is given by:

$$x(t;\, x^o,\, t_o) = \Phi(t,\, t_o)x^o \ \forall\, t \text{ , } \forall\, x^o . \tag{4-5}$$

Proof

Using (4-4), (4-5) reduces to x^o for $t = t_o$. Again differentiating (4-5), we observe that it satisfies the differential equation (4-2). Q.E.D.

The matrix $\Phi(t,t_o)$ is called the state transition matrix as it is a linear transformation which maps the state x^o at t_o into the state $x(t)$ at time t . The state transition matrix has the group property $\Phi(t_3,\, t_2)\, \Phi(t_2,\, t_1) = \Phi(t_3,\, t_1)$ $\forall\, t_1$, t_2 , t_3 . An immediate consequence [17] of this property is $\Phi^{-1}(t_1,\, t_2) = \Phi(t_2,\, t_1)$.

The additional effect on the state vector of the control function $u(t)$ is developed as follows:

Theorem (4.6)

Consider the differential equation (4-1) under Assumption A1. The solution that goes through the state x^o at t^o is given by:

$$x(t) = x(t;\, x_o,\, t_o,\, u[t_o,\, t]) = \Phi(t,\, t_o)x^o + \int_{t_o}^{t} \Phi(t,\, s)B(s)u(s)ds . \tag{4-6}$$

Proof

The initial condition could be verified directly. Differentiation of (4-6) and direct substitution into (4-1) proves the result noting that

$$\frac{d}{dt}\int_{t_o}^{t} \Phi(t, s)B(s)u(s)ds = \Phi(t, t)B(t)u(t) + \int_{t_o}^{t} \frac{d}{dt}\Phi(t, s)B(s)u(s)ds$$

$$= B(t)u(t) + A(t)\int_{t_o}^{t} \Phi(t, s)B(s)u(s)ds$$

and

$$\frac{d}{dt}\Phi(t, t_o)x^o = A(t)\Phi(t, t_o)x^o \; .$$

Q.E.D.

If $A(t) = A$ is constant, then the state transition matrix is $\Phi(t, t_o) = e^{A(t-t_o)}$ where by definition $e^A = I + \sum_{m=1}^{\infty} \frac{A^m}{m!}$; and (4-6) reduces to

$$x(t) = e^{At}x^o + \int_{t_o}^{t} e^{A(t-s)}B(s)u(s)ds \; . \qquad (4\text{-}6a)$$

Any control function $u \in \Omega$ is called an admissible control for the linear system. If for given x^o and x_i^T, $i = 1, 2, \ldots, n$, there exists at least one control $u \in \Omega$ such that the solution (4-6) satisfies the condition $x_i(T) = x_i^T$ for $i = 1, 2, \ldots, n$, then the optimization problem is feasible and the linear system is termed controllable. An admissible control for which the problem is feasible will be called a feasible control. Among the feasible controls, if $u^* \in \Omega$ minimizes $x_o(T)$ then it is called an optimum control and the corresponding solution $x^*(t)$, $u^*(t)$, $t_o \leqq t \leqq T$, is called an optimum solution to the optimization problem (4-1).

Denoting by $S_T(x^o)$ the set of reachable points at time T , starting from x^o at t_o and using an admissible control $u \in \Omega$, it may be noted that

$$S_T(x^o) = \left\{ x(T) \;\middle|\; x(T) = \Phi(T, t_o)x^o + \int_{t_o}^{T} \Phi(T, \tau)B(\tau)u(\tau)d\tau \atop u \in \Omega \right\} . \qquad (4\text{-}7)$$

Similarly, the set of reachable points at each t, $t_o \leqq t \leqq T$, may be denoted by $S_t(x^o)$.

It is then evident that the system is controllable and the optimization problem (4-1) is feasible if and only if for some value of $x_o(T)$,

$$\left(x_o(T) \; , \; x_1^T \; , \; \ldots , \; x_n^T\right) \in S_T(x^o) \; .$$

The terminal conditions of (4-1) may be generalized by allowing $x^o(T) \in X^o$, $(x_1(T) \; , \; \ldots , \; x_n(T)) \in X^T$ where $X^o \subset E^{n+1}$ and $X^T \subset E^n$ are compact convex sets.

The definition of $S_T(x^o)$ may also be generalized to the set $S_T(X^o)$ as the set of reachable points at time T , starting from any point of $X^o \subset E^{n+1}$, and using only admissible controls $u \in \Omega$.

Under Assumptions A1, A2, and A3 (page 24), the set $S_T(X^o)$ is closed and bounded for each t, $t_o \leq t \leq T$. Boundedness of $S_T(X^o)$ could be proved directly from the definition (4-7) and the assumptions. The proof of closure could be found in [18]. The fact that the set $S_T(X^o)$ is convex under certain conditions as expressed in the following theorem is also a matter of importance.

Theorem (4.8)

Under the assumptions A1, A2, and A3, the set $S_T(X^o)$ is convex, if X^o is convex.

Proof

Let x_T^1 and $x_T^2 \in S_T(X^o)$; i.e., they are the respective solutions of (4-1) with admissible control vectors u^1, $u^2 \in \Omega$ and initial points x^{o1} and x^{o2}, respectively. For $0 \leq \lambda \leq 1$, consider the point $x_T^\lambda = \lambda x_T^1 + (1 - \lambda)x_T^2$. The problem is to prove that $x_T^\lambda \in S_T(X^o)$. Now

$$S_T(X^o) = \left\{ x \mid x = \Phi(T, t_o)x^o + \int_{t_o}^{T} \Phi(T, s)B(s)u(s)ds \ , \ x^o \in X^o \ , \ u \in \Omega \right\}$$

and hence

$$x_T^\lambda = \Phi(T, t_o)[\lambda x^{o1} + (1 - \lambda)x^{o2}] + \int_{t_o}^{T} \Phi(T, s)B(s)[\lambda u^1(s) + (1 - \lambda)u^2(s)]ds \ .$$

But since X^o and $P(t)$ are both convex, this reduces to

$$x_T^\lambda = \Phi(T, t_o)x^{o\lambda} + \int_{o}^{T} \Phi(T, s)B(s)u^\lambda(s)d\tau$$

where $x^{o\lambda} = \lambda x^{o1} + (1 - \lambda)x^{o2} \in X^o$ and

$$u^\lambda(s) = \lambda u^1(s) + (1 - \lambda)u^2(s) \in P(s) \ , \ t_o \leq s \leq T \ .$$

Hence $x_T^\lambda \in S_T(X^o)$. Q.E.D.

It is noteworthy that in the above proof t, $t_o \leq t \leq T$ could replace T and hence $S_t(X^o)$ is convex for all $t \in [t_o, T]$ if X^o is convex. The compactness and convexity properties obviously are true when the set X^o degenerates to a single point $x^o \in E^{n+1}$. The above theorem holds for an arbitrary compact Ω, which need not be convex [19, p. 164-168].

It is necessary to establish the following theorem which characterizes the optimal trajectory.

Theorem (4.9)

If for a solution $x^*(t)$ of $dx(t)/dt = A(t)x(t) + B(t)u(t)$, $u \in \Omega$, $x(o) \in X^o$, $x^*(T)$ belongs to the boundary of $S_T(X^o)$, then $x^*(t)$ belongs to the boundary of $S_t(X^o)$ for $t_o \leq t \leq T$.

Proof

On the contrary, suppose $x^*(t_1)$ is an interior point of $S_{t_1}(X^o)$. Let R_{t_1}: E^{n+1} map the points $x = x(t_1)$ of the solutions into their values at $t = T$, $x(T)$, using the same control as used for $x^*(t)$. Let U be any neighborhood of $x^*(t_1)$ and let $U \subset S_{t_1}(X^o)$. Clearly, $V = R_{t_1}(U) \subset S_T(X^o)$. But the inverse function $R_{t_1}^{-1}$ is continuous and hence V is a neighborhood of $x^*(T)$ contained in $S_T(X^o)$ which is a contradiction since $x^*(T)$ is a boundary point of $S_T(X^o)$ by hypothesis. Q.E.D.

In the following section it is proved that for $x^*(t)$ to be an optimal solution to (4-1), $x^*(T)$ must be a boundary point of $S_T(X^o)$. Hence the above theorem establishes the property that the optimum solution $x^*(t)$ is an *extremal solution*, i.e., belongs to the boundary of $St(X^o)$ for $t_o \leq t \leq T$. This property obviously holds when X^o degenerates to a single point $x^o \in E^{n+1}$.

THE MINIMUM PRINCIPLE FOR LINEAR OPTIMAL CONTROL PROBLEM

With the characterization of the set $S_T(X^o)$ of reachable points, wherein the terminal point $x(T)$ must lie for feasibility, the original minimization problem (4-1) may be given an equivalent *geometric* definition (see Figure 5).

Find the lowest point in the nonempty set $L \cap S_T(x^o)$ where the line L is given by:

$$L = \left\{(x_o, x_1, \ldots, x_n) \mid x_1 = x_1^T, \ldots, x_n = x_n^T\right\} .$$

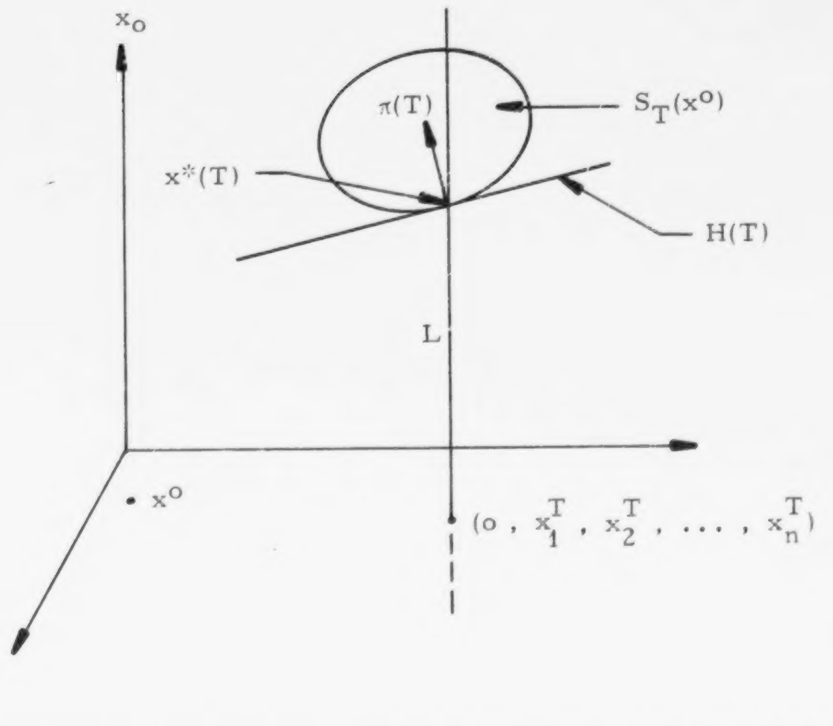

FIGURE 5. GEOMETRIC REPRESENTATION OF THE MINIMIZATION PROBLEM

In the above, the increasing x_o-direction is considered "up." Obviously, for the problem (4-1) to be feasible, the set $L \cap S_T(x^o)$ must be nonempty, which is the case when the process is controllable. Since $S_T(x^o)$ is closed, bounded, and convex, if (4-1) is feasible, $x^*(T)$, the lowest point of $L \cap S_T(x^o)$, must be a boundary point of $S_T(x^o)$.

From the well-established theory of convex sets [20], it is known that there exists a supporting hyperplane $H(T)$ passing through $x^*(T)$ such that the interior of $S_T(x^o)$ lies entirely on one side of this hyperplane. $H(T)$ may be expressed by its unit normal vector $\pi(T)$ as $\pi(T)x + \mu = 0$ where μ is a scalar and $\pi(T)$ is directed into $S_T(x^o)$, i.e., it points into a half space defined by $H(T)$ that also contains $S_T(x^o)$.

Then for all $x \in S_T(x^o)$,

$$\pi(T)x + \mu \geqq 0 ,$$

whereas for $x^*(T)$ at the boundary of $S_T(x^o)$,

$$\pi(T)x^*(T) + \mu = 0 ,$$

in which $x^*(T)$ is the optimal terminal point for (4-1) and minimizes the value of $x_o(T)$ among all $x(T) \in L \cap S_T(x^o)$.

Hence,

$$\pi(T)[x - x^*(T)] \geqq 0 \qquad x \in S_T(x^o) . \qquad (4\text{-}10)$$

If $u \in \Omega$ and $u^* \in \Omega$ are the respective control functions which transfer the system to x and $x^*(T)$ at time T , from the initial position x^o at t_o , then using (4-6) and (4-10), Equation (4-11) results.

$$\pi(T) \left[\int_{t_o}^{T} \Phi(T, s)B(s)\{u(s) - u^*(s)\}ds \right] \geqq 0 . \qquad (4\text{-}11)$$

Consider next the adjoint system of (4-2) described by the following system of differential equations.

$$\frac{d\pi(t)}{dt} = -\pi(t)A(t), \quad t_o \leqq t \leqq T \qquad (4\text{-}12)$$

in which $\pi(t)$ is a $(n + 1)$-row vector.

The importance and usefulness of the adjoint system is based on the following lemma.

Lemma (4.12a)

Let $x(t)$ and $\pi(t)$ be any solutions of (4-2) and (4-12), respectively. Then

$$\pi(t)x(t) \equiv \text{constant}.$$

Proof

$$\frac{d}{dt}[\pi(t)x(t)] = \frac{d\pi(t)}{dt}x(t) + \pi(t)\frac{dx(t)}{dt}$$

$$= -\pi(t)A(t)x(t) + \pi(t)A(t)x(t) = 0 .$$

Hence $\pi(t)x(t) \equiv$ constant. Q.E.D.

Equation (4-12) also serves as an adjoint system to Equation (4-1) and plays a very important role in characterizing an optimum solution to (4-1), as evident from the two following theorems.

Theorem (4.13)

In order for $x^*(t)$, $t_o \leqq t \leqq T$ to be an optimum solution of (4-1), there must exist a nontrivial solution $\pi(t)$ of the adjoint system (4-12) such that

$$\pi(t)x^*(t) = \min_{x \in S_t(x^o)} \pi(t)x \text{ for all } t,\ t_o \leqq t \leqq T .$$

Proof

Let $u^*(t)$ be the corresponding control for the solution $x^*(t)$. Suppose for $t = t_1$, $x^1(t_1) \in S_{t_1}(x^o)$. Now consider the points $x^1(T) = x(T;\ t_1,\ x^1(t_1)\ ,\ u^*[t_1,\ T])$ and $x^*(T) = x(T;\ t_1,\ x^*(t_1)\ ,\ u^*[t_1,\ T])$ where these are the terminal points at T when the same control u^* is applied during $[t_1, T]$ to the system starting from $x^1(t_1)$ and $x^*(t_1)$, respectively. From (4-6),

$$x^1(T) = \Phi(T,\ t_1)x^1(t_1) + \int_{t_1}^{T} \Phi(T,\ s)B(s)u^*(s)ds$$

and

$$x^*(T) = \Phi(T,\ t_1)x^*(t_1) + \int_{t_1}^{T} \Phi(T,\ s)B(s)u^*(s)ds .$$

Because $x(T;\ t_1,\ x^1(t_1)\ ,\ u^*[t_1,\ T]) \in S_T(x^o)$, it follows from (4-11) that

$$\pi(T)[x^1(T) - x^*(T)] \geqq 0 .$$

Using the above relations, the relationship reduces to

$$\pi(T)\Phi(T,\ t_1)[x^1(t_1) - x^*(t_1)] \geqq 0 . \qquad (4\text{-}14)$$

It may be noted that $\pi(t) = \pi^o\Phi^{-1}(t,\ t_o)$ is a solution for the adjoint system (4-12), where $\Phi^{-1}(t,\ t_o) = \Phi(t_o,\ t)$, defined in Theorem (4.3), and $\pi^o = \pi(t_o)$ is a constant $(n + 1)$-vector. This formula for $\pi(t)$ can be verified to be a solution of (4-12) by direct differentiation. If $\pi^o \neq 0$, then $\pi(t)$ is a nontrivial solution of the adjoint equation, i.e., $\pi(t)$ vanishes nowhere on $t_o \leqq t \leqq T$.

Using the above solution,

$$\pi(T)\Phi(T,\ t_1) = \pi^o\Phi^{-1}(T,\ t_o)\Phi(T,\ t_1) = \pi^o\Phi^{-1}(t_1,\ t_o) = \pi(t_1) .$$

Hence, (4-14) reduces to

$$\pi(t_1)[x^1(t_1) - x^*(t_1)] \geqq 0 \text{ for all } t_1\ ,\ t_o \leqq t_1 \leqq T \qquad (4\text{-}15)$$

or

$$\pi(t)x^*(t) = \min_{x \in S_t(x^o)} \pi(t)x .$$

Q.E.D.

Finally, it remains to prove the celebrated Maximum Principle [15] for the linear optimal control problem. This is stated in an equivalent form in the following theorem.

Theorem (4.16)

Suppose that $u^*(t) \in P(t)$, $t_o \leqq t \leqq T$, is an admissible control and such that the corresponding trajectory $x^*(t)$ satisfies

$$x^*(o) = x^o$$

$$x_i^*(t) = x_i^T , \quad i = 1, 2, \ldots, n$$

$$\frac{dx^*(t)}{dt} = A(t)x^*(t) + B(t)u^*(t)$$

almost everywhere (a.e.) in t , $t_o \leqq t \leqq T$.

Then, in order for $u^*(t)$ and $x^*(t)$ to be optimal for (4.1), i.e., to minimize $x_o(T)$, it is necessary that there exists a nontrivial solution $\pi(t)$ of the adjoint system (4-12) such that for almost all $t \in [t_o, T]$,

$$\pi(t)B(t)[u(t) - u^*(t)] \geqq 0 \text{ for all } u(t) \in P(t) . \tag{4-17a}$$

Furthermore,

$$\pi_o(t) \geqq 0 , \quad t_o \leqq t \leqq T . \tag{4-17b}$$

Proof

Assume that $u^*(t)$ on $t_o \leqq t \leqq T$ is optimal for (4-1) and transfers x^o to $x^*(T)$, a boundary point of $S_T(x^o)$, and

$$x^*(t) = \Phi(t, t_o)x^o + \int_{t_o}^{t} \Phi(t, s)B(s)u(s)ds$$

$$= \Phi(t, t_o)x^o + \Phi(t, t_o) \int_{t_o}^{t} \Phi^{-1}(s, t_o)B(s)u(s)ds .$$

Let $\pi(T)$ be the unit normal vector to the supporting hyperplane $H(T)$ to $S_T(x^o)$ at $x^*(T)$.

Define a nontrivial (for $\pi^o \neq 0$) solution $\pi(t) = \pi^o\Phi^{-1}(t, t_o)$ to the adjoint system (4-12) with $\pi(T) = \pi^o\Phi^{-1}(T, t_o)$. Computing the inner product of $\pi(t)$ and $x^*(t)$:

$$\pi(t)x^*(t) = \pi^o x^o + \int_{t_o}^{t} \pi^o\Phi^{-1}(s, t_o)B(s)u(s)ds = \pi^o x^o + \int_{t_o}^{t} \pi(s)B(s)u(s)ds .$$

Now suppose that $\pi(t)B(t)u^*(t) > \min\limits_{u(t)\in P(t)} \pi(t)B(t)u(t)$ on some set of positive duration in $t_o \leqq t \leqq T$. Define the control $\hat{u} \in \Omega$ on $t_o \leqq t \leqq T$ such that

$$\pi(t)B(t)\hat{u}(t) = \min_{u(t)\in P(t)} \pi(t)B(t)u(t) .$$

It can be shown that $\hat{u}(t)$ can be chosen to be measureable [19]. But for the corresponding solution $\hat{x}(t)$ to $\hat{u}(t)$,

$$\pi(T)\hat{x}(T) = \pi^o x^o + \int_{t_o}^{T} \pi(s)B(s)\hat{u}(s)ds \ .$$

Since

$$\int_{t_o}^{T} \pi(s)B(s)u^*(s)ds > \int_{t_o}^{T} \pi(s)B(s)\hat{u}(s)ds$$

$\pi(T)x^*(T) > \pi(t)\hat{x}(T)$ in which $\hat{x}(T) \in S_T(x^o)$ as $\hat{u} \in \Omega$. This contradicts Theorem (4.13). Hence $\pi(t)B(t)[u(t) - u^*(t)] \geqq 0$ for all $u(t) \in P(t)$ for almost all $t \in [t_o, T]$.

To prove that $\pi_o(t) \geqq 0$, consider the set $S_t^+(x^o)$ defined by

$$S_t^+(x^o) = \{x \mid x_o(t) \geqq \tilde{x}_o(t) \ , \ x_i(t) = \tilde{x}_i(t) \ ,$$

$$i = 1, 2, \ldots, n \text{ for some } \tilde{x}(t) \in S_t(x^o)\} \ .$$

It may be noted that for minimizing $x_o(T)$, it is equivalent to consider the set $S_t^+(x^o)$ in place of $S_t(x^o)$ and (4-10) holds for all $x \in S_t^+(x^o)$. Now consider the point $\bar{x}(t) \in S_t^+(x^o)$ given by $\bar{x}(t) = (\bar{x}_o(t) \ , \ x_1^*(t) \ , \ \ldots, \ x_n^*(t))$ where $\bar{x}_o(t) - x_o^*(t) = \delta > 0$.

As $\bar{x}(t)$, $x^*(t) \in S_t^+(x^o)$, it follows from (4-10) that

$$\pi(t)[\bar{x}(t) - x^*(t)] \geqq 0$$

in which $x^*(t) = (x_o^*(t) \ , \ x_1^*(t) \ , \ \ldots, \ x_n^*(t))$. Hence $\pi_o(t)[\bar{x}_o(t) - x_o^*(t)] \geqq 0$ or $\pi_o(t)\delta \geqq 0$. As $\delta > 0$, so $\pi_o(t) \geqq 0$. Q.E.D.

Note: If the differential equation in (4-1) is given by

$$\frac{dx(t)}{dt} = A(t)x(t) + B(t)u(t) + d(t) \text{ for } t_o \leqq t \leqq T \qquad (4\text{-}1a)$$

where $d(t)$ is a $(n + 1)$-vector function continuous on $[t_o, T]$, all preceding results and those to be presented in the following two sections of this chapter will still hold with $B(t)u(t)$ being replaced by $B(t)u(t) + d(t)$.

TRANSVERSALITY CONDITIONS

Transversality conditions for the initial and terminal end points may be easily obtained for the variable end-point optimization problem obtained from (4-1). These conditions are required when the initial and final states are specified to lie in given sets in the state space, but their exact locations are not given.

Theorem (4.18)

For the generalized version of Problem (4-1) with $x(t_o) \in X^o \subset E^{n+1}$ and $(x_1(T), \ldots, x_n(T)) \in X^T \subset E^n$, Theorems (4.13) and (4.16) are valid and moreover $\pi(t)$ can be chosen such that:

a. $\pi(T)[x - x^*(T)] \leq 0$ for all $x = (x_o^*(T), x_1, x_2, \ldots, x_n)$ where $(x_1, x_2, \ldots, x_n) \in X^T$ and

b. $\pi(0)[x - x^*(0)] \geq 0$ for all $x \in X^o$

whenever both X^o and X^T are compact and convex subsets of E^{n+1} and E^n , respectively.

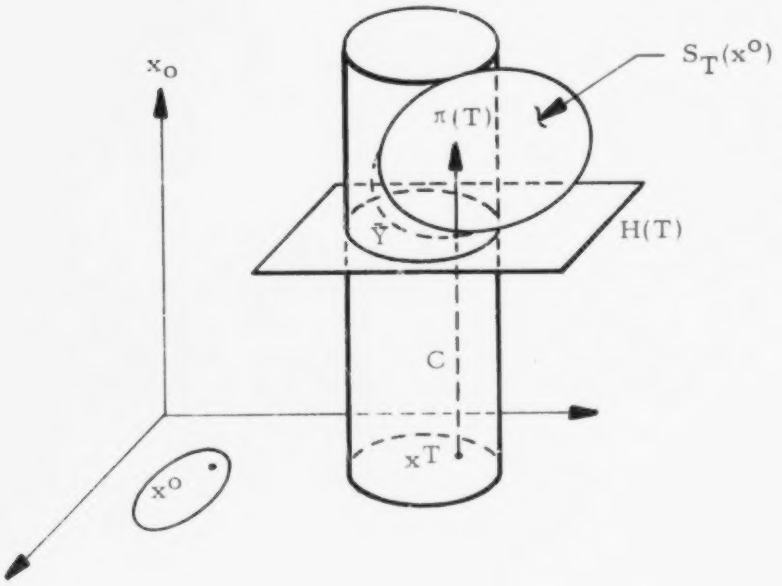

FIGURE 6. GEOMETRY OF THE GENERALIZED PROBLEM WITH VARIABLE TERMINAL POINTS

Proof

Given an optimal trajectory for the variable terminal point problem, it must also solve the fixed terminal point problem (4-1) with $x^o = x^*(0)$, $x_i^T = x_i^*(T)$, $i = 1, 2, \ldots, n$ and hence Theorem (4.16) is valid.

From Theorem (4.8) the set $S_T(X^o)$ is convex if X^o is and the proof of Theorem (4.13) goes through with $S_T(X^o)$ replacing $S_T(x^o)$.

a. From Theorem (4.13), the expression for the initial end point is obtained:

$$\pi(0)[x - x^*(0)] \geq 0 \text{ for all } x \in X^o \text{ as } S_o(X^o) \equiv X^o .$$

b. Considering the geometry of the generalized problem (see Figure 6), the line L (page 27) now becomes the convex cylinder C given by

$$C = \{(x_o, x_1, \ldots, x_n) \mid (x_1, x_2, \ldots, x_n) \in X^T\} .$$

The object is to find the lowest point $x^*(T)$ in the nonempty set $Z = C \cap S_T(X^o)$. Z is compact and convex; and it may be noted that for all $x \in Z$, $x_o \geq x_o^*(T)$.

Consider the following sets:

$Y = \{x \mid x_o \leq x_o^*(T) , (x_1, \ldots, x_n) \in X^T\}$ and

$\bar{Y} = \{x \mid x_o = x_o^*(T) , (x_1, \ldots, x_n) \in X^T\}$.

As for all $x \in Y \cap Z$ we have $x_o \equiv x_o^*(T)$, $H(T)$ given by $\pi(T)x + \mu = 0$ is a separating hyperplane which separates the nonempty convex sets Y and Z, where

$$\pi(T) = (1, 0, 0, \ldots, 0) \text{ and } \mu = x_o^*(T) .$$

Hence,

$$\inf \{\pi(T)x + \mu \mid x \in Z\} \geqq \sup \{\pi(T)x + \mu \mid x \in Y\}$$

or

$$\pi(T)x^*(T) + \mu \geqq \{\pi(T)x + \mu \mid x \in \overline{Y}\}$$

or

$$\pi(T)[x - x^*(T)] \leqq 0 \quad \text{for all} \quad x \in \overline{Y} . \qquad \text{Q.E.D.}$$

The transversality conditions could be generalized if $X^o \subset E^p$ and $X^T \subset E^q$ where $2 < p \leqq n + 1$ and $1 < q \leqq n$, and provide the extra conditions needed to obtain the optimal initial and terminal end points. If one of these end points is fixed, only one condition is required.

LINEAR OPTIMAL CONTROL PROBLEM WITH STATE VARIABLE CONSTRAINTS

In the optimization problem (4-1), only the control vector u was constrained to lie in the set Ω . However, often due to physical limitations the state variable x may be constrained to be in a closed subset $\Lambda \subset E^{n+1}$. These constraints may involve both the state and control vectors explicitly or the state vector alone, the latter case being more difficult to handle. Solution methods for these cases are available, e.g., in [21] and [22].

For the present purpose it is appropriate to consider below linear state variable constraints as represented by a system of linear inequalities and involving only the state variables. Such constraints may be represented by

$$G(x, t) \leqq 0 \tag{4-19}$$

in which $G(x, t)$ is a vector-valued linear function of $x(t)$, and t. $G(x, t) = 0$ represents the smooth boundary of the closed convex region $\Lambda \subset E^{n+1}$. Only those control functions $u \in \Omega$ are now *admissible* which give trajectories $x(t)$ in Λ . For compact and convex Ω and X^o , it can be shown that the new set of attainability $S_T^\Lambda(X^o) \subset \Lambda$, using admissible controls, is again a compact convex set and the optimal trajectory $x^*(t)$ must lead to a boundary point $x^*(T)$ of $S_T^\Lambda(X^o)$.

The optimal trajectory in this case may consist of two types of segments — *interior* segments and *boundary* segments. The interior segments form the segments of the optimal trajectory which (except for the end points) wholly lie in the interior of the feasible region defined by the state variable constraints. The boundary segments are the segments of the optimal trajectory on the boundary of the closed feasible region where one or more of the state variable constraints are active. The interior segments satisfy Theorem (4.16) which is equivalent to the Maximum Principle. The boundary segments follow a modified Maximum Principle [15, Chapter VI] and the control variable on the boundary is determined by the state variable constraints. At junction points, where the optimal trajectory either enters or leaves the constraint boundary, special jump conditions [22] must be satisfied by the solution of the adjoint system (4-12). In the following theorem only those results are presented that are required in developing a solution to the Dispersion Model.

Theorem (4.20)

In order for u^* and x^* to be optimum solutions for the linear optimal control problem (4-1) with state variable constraints represented by (4-19), the following are necessary:

a. Each interior segment of $x^*(t)$ will satisfy Theorem (4.16).

b. On each point of the boundary segment, $d^kG(x, t)/dt^k = 0$ for $k = 0, 1, \ldots, q$ where q is the lowest derivative of $G(x)$ explicitly involving the control vector.† At the entering corner t_1 of a boundary segment this result holds for $k = 0, 1, \ldots, q-1$.

Proof

a. First, assume that $x^*(t)$, $t \in [t_1, t_2]$ is an interior segment of the optimal trajectory, with $x^*(t_1) = x^{t_1}$ and $x^*(t_2) = x^{t_2}$. From the Principle of Optimality, it may be observed that in order for $x^*(t)$ to be the optimal trajectory for $t \in [0, T]$, the interior segment $x^*(t)$, $t \in [t_1, t_2]$ must be optimal among all such segments which transfer the system from x^{t_1} at t_1 to x^{t_2} at t_2 using admissible controls. Otherwise by changing this segment there results a better optimal trajectory for $[0 , T]$. Hence $x^*(t)$, $t \in [t_1, t_2]$ must satisfy Theorem (4.16).

b. Since the constraint function $G(X)$ must vanish identically when the solution lies on the constraint boundary, it follows that its derivatives with respect to t must also vanish on the constraint boundary. At the entering corner, for the same reason, $d^kG(x, t_1)/dt^k = 0$ for $k = 0, 1, 2, \ldots, q-1$, and these play the role of terminal constraints for the unconstrained segment preceding the boundary segment. $d^qG(x, t)/dt^q = 0$ determines the optimum control vector on the boundary. At the entering corner for $t = t_1$ the control vector may be undefined as it may switch to a new value for $t > t_1$ and only the first $q-1$ derivatives are used.

SOLUTION OF THE DISPERSION MODEL

In Chapter II, several models were conceived with a view to optimize the dispersive process of polluting substances in the receiving waters and specify optimal discharge plans to meet desired quality objectives. In this section, the optimal control theory and the related maximum principle, discussed above, are applied to obtain solutions for the continuous dispersion models. For this purpose, they are first formulated in a convenient form suitable for the application of the maximum principle with certain changes in the notations. Discussion of this may well begin with the solution of Problem B which embodies the more practicable "standards approach" to water quality control.

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†In the sense of Bryson, Denham, and Dreyfus [21] this means that the state variable constraint is of q^{th} order. We assume here that $G(x, t)$ is differentiable at least q times in t .

Problem B

In Chapter II, Problem B has been expressed as:

$$\text{Find } D = \max \int_0^L S(x)dx \ , \ S(x) \in S^{**} \text{ and the corresponding optimal } S(x), \qquad (2\text{-}19)$$

where S^{**} is the set of feasible discharge patterns $S(x)$ satisfying the following equations:

$$\frac{dc_s(x)}{dx} = a(x)c_s(x) - b(x)\int_0^x S(y)dy - T_o b(x) \ , \ x \in [0 \ , \ L] \qquad (2\text{-}16)$$

$$0 \leq L_s(x) \leq S(x) \leq U_s(x) \ , \ x \in [0 \ , \ L] \qquad (2\text{-}20)$$

$$0 \leq c_s(x) \leq U_c(x) \ , \ x \in [0 \ , \ L] \ . \qquad (2\text{-}21)$$

The following substitutions are in order:

$$t = x \ ; \qquad T = L$$

$$x_1(t) = c_s(x) \ ; \qquad x_o(t) = -\int_0^x S(x)dx$$

$$u(t) = S(x); \qquad F = T_o \ .$$

For simplicity it is also assumed that

$$L_s(t) \equiv \underline{u}, U_s(t) \equiv \bar{u} \ , \ t \in [0 \ , \ T] \qquad (4\text{-}21)$$

and

$$U_c(t) \equiv \bar{c} \ \forall \ t \in [0 \ , \ T] \ . \qquad (4\text{-}22)$$

If maximum allowable concentration and/or bounds on discharge rate vary from section to section, minor changes of the model can be made.

With the substitutions, Problem B now becomes

Minimize $\quad x_o(T)$

$$\text{Subject to } \frac{dx_o(t)}{dt} = \qquad\qquad - u(t) \qquad (4\text{-}23)$$

$$\frac{dx_1(t)}{dt} = b(t)x_o(t) + a(t)x_1(t) \qquad - b(t)F \qquad (4\text{-}24)$$

almost everywhere on $[0 \ , \ T]$ and

$$0 \leq x_1(t) \leq \bar{c} \ \forall \ t \in [0 \ , \ T] \qquad (4\text{-}25)$$

$$0 \leq \underline{u} \leq u(t) \leq \bar{u} \ \forall \ t \in [0 \ , \ T] \ . \qquad (4\text{-}26)$$

If it is expressed in the form of (4-1) we have for $t \in [0 \ , \ T]$, $u(t) \equiv u(t)$,

$$x(t) = \begin{vmatrix} x_o(t) \\ x_1(t) \end{vmatrix} \quad A(t) = \begin{vmatrix} 0 & 0 \\ b(t) & a(t) \end{vmatrix} \quad B(t) = \begin{vmatrix} -1 \\ 0 \end{vmatrix} \quad d(t) = \begin{vmatrix} 0 \\ -b(t)F \end{vmatrix} \ .$$

The initial and terminal conditions are given by:

$$x_o(0) = 0 \quad \text{and} \quad x_1^T = 0 \; . \tag{4-27}$$

This may be expressed by

$$x(0) \in X^o = \{x \mid x_o = 0\} \quad \text{and} \quad x_1(T) = x_1^T = 0 \; .$$

Thus the problem involves a variable initial point but fixed terminal point.

Problem B as expressed above is a linear optimal control problem with a state variable constraint (4-25).

To determine if this constraint is active, the problem will be solved at first ignoring this constraint. Let $\bar{x}_1 = \max_{t \in [0,T]} [x_1(t)]$ for the modified problem. If $\bar{x}_1 \leq \bar{c}$, the constraint (4-25) is inactive, and the solution ignoring (4-25) represents the solution of Problem B. Otherwise (i.e., if $\bar{x}_1 > \bar{c}$), the original problem with the state variable constraint must be solved. The physical nature of the problem suggests that if there is no upper bound to the concentration level (i.e., (4-25) is absent) the optimal solution would be to discharge as much as possible, i.e., $u(t) = \bar{u} \; \forall \; t \in [0 , T]$. This result may be formalized using the maximum principle as follows.

Solution of Problem B without State-Variable Constraint

Assume that $a(t)$ and $b(t)$ are continuous on $[0 , T]$. This assumption is reasonable because $a(t) = v(t)/E(t)$ and $b(t) = 1/A(t)E(t)$ and the cross-sectional area $A(t)$, velocity $v(t)$ and dispersion coefficient $E(t)$ may be considered continuous on $[0 , T]$. Hence, $A(t)$ and $d(t)$ are continuous, $B(t)$ is constant, $P(t) = [\underline{u} , \bar{u}]$ and $\Omega = \{u : u(t) \in [\underline{u} , \bar{u}] , t \in [0 , T]\}$. Problem B also satisfies assumptions A1-A3 (page 24).

Applying Theorem (4.16) it develops that for x^* and u^* to be optimal solutions for Problem B, it is necessary that the adjoint system $d\pi(t)/dt = -\pi(t)A(t)$ have a solution $\pi(t)$ such that, $\pi_o(t) \geq 0$ and

$$\pi(t)B(t)u^*(t) = \min_{u(t) \in P(t)} \pi(t)B(t)u(t) \tag{4-28}$$

for almost all $t \in [0 , T]$ where

$$\pi(t)B(t)u(t) = [\pi_o(t), \pi_1(t)] \begin{bmatrix} -1 \\ 0 \end{bmatrix} u(t) = -\pi_o(t)u(t) \; .$$

The adjoint system for Problem B is given by:

$$\begin{aligned} \frac{d\pi_o(t)}{dt} + \pi_1 b(t) &= 0 \\ \frac{d\pi_1(t)}{dt} + \pi_1 a(t) &= 0 \; . \end{aligned} \tag{4-29}$$

Solving the two differential equations it results that

$$\pi_1(t) = k_1 e^{-\int_0^t a(s)ds}$$

in which k_1 is a constant of integration and

$$\pi_o(t) = k_2 - k_1 \int_0^t \left[b(s) e^{-\int_0^s a(y)dy} \right] ds \tag{4-30}$$

where k_2 is a constant of integration. If $a(t) \equiv a$ and $b(t) \equiv b$ for all $t \in [0\ ,\ T]$ we get

$$\pi_1(t) = k_1 e^{-at} \quad \text{and} \quad \pi_o(t) = k_2 + k_1 \frac{b}{a} e^{-at} \, . \qquad (4\text{-}30a)$$

Transversality condition (Theorem 4.18) applied to the free initial point gives us

$$\pi(0)[x - x^*(0)] \geqq 0 \quad \text{for all} \quad x \in X^0 = \{x \mid x_o = 0\}$$

which reduces to

$$[\pi_o(0),\ \pi_1(0)] \begin{bmatrix} 0 \\ x_1(0) - x_1^*(0) \end{bmatrix} \geqq 0 \quad \text{or}$$

$$\pi_1(0)[x_1(0) - x_1^*(0)] \geqq 0 \, . \qquad (4\text{-}31)$$

(4-31) is satisfied for all $x_1(0)$ only if $\pi_1(0) = 0$.

From (4-30) this implies $k_1 = 0$ and, finally,

$$\pi_1(t) \equiv 0 \ \text{and} \ \pi_o(t) = k_2 \ \forall \ t \in [0\ ,\ T] \, . \qquad (4\text{-}32)$$

But $\pi_o(T) = k_2 \geqq 0$ from Theorem (4.16) and the minimum principle (4.28) reduces to

$$- k_2 u^*(t) = \min_{u(t) \in P(t)} - k_2 u(t) \ \text{for all} \ t \in [0\ ,\ T] \, . \qquad (4\text{-}33)$$

Hence, the optimal value of the control variable is given by $u^*(t) \equiv \bar{u}$ for all $t \in [0\ ,\ T]$.

The optimal concentration profile $x_1(t)$ is obtained by using this value of $u(t)$. From (4-23), $x_o^*(t) = -\bar{u}t$ for all $t \in [0\ ,\ T]$ as $x_o(0) = 0$. Substituting this in (4-24) we have

$$\frac{dx_1^*(t)}{dt} = a(t)x_1^*(t) - b(t)\bar{u}t - b(t)F \, . \qquad (4\text{-}34)$$

Integrating (4-34) we obtain

$$x_1^*(t)e^{-\int_0^t a(y)dy} = \omega_1 - \int_0^t \left[b(s)(\bar{u}s + F)e^{-\int_0^s a(y)dy} \right] ds \, . \qquad (4\text{-}35)$$

ω_1 being the constant of integration and

$$\omega_1 = \int_0^T \left[b(t)(\bar{u}t + F)e^{-\int_0^t a(y)dy} \right] dt \qquad (4\text{-}36)$$

which satisfies the boundary condition $x_1(T) = 0$.

This is the complete general solution of Problem B ignoring the state variable constraint. To proceed further it is necessary to know the actual forms for the functions $a(t)$ and $b(t)$. Once these functions are known from the hydrological characteristics of the estuary, (4-35) and (4-36) provide the optimum concentration profile $x_1^*(t)$. The value of $\bar{x}_1 = \max x_1^*(t)$ may be obtained by analytical or numerical means. $x_1^*(t)$ is a continuous function and differentiable if a(t) and b(t) are simple algebraic functions. If $\bar{x}_1 > \bar{c}$, then the state variable constraint is active and one must proceed to the solution of the control problem with state variable constraint.

Constant Coefficients Case (A1, Table I)

In this case $a(t) \equiv a$; $b(t) \equiv b$ for all $t \in [0\ ,\ T]$ as the result of both the volume flow Q(t) and the area A(t) being constant.

As $e^{-\int a(t)dt} = e^{-at}$, from (4-35) and (4-36), by integration:

$$x_1^*(t) = \frac{b}{a}\left\{\bar{u}\left(t + \frac{1}{a}\right) + F\right\} - \frac{b}{a}\left\{\bar{u}\left(T + \frac{1}{a}\right) + F\right\} e^{a(t-T)} \qquad (4\text{-}37)$$

for $t \in [0\ ,\ T]$ and the initial concentration

$$x_1^*(0) = \frac{b}{a}\left\{\frac{\bar{u}}{a} + F\right\} - \frac{b}{a}\left\{\bar{u}\left(T + \frac{1}{a}\right) + F\right\} e^{-aT} .$$

Solution of Problem B with State-Variable Constraints

As discussed in the preceding Section (page 33), the optimal trajectory in this case may consist of two types of segments — interior segments and boundary segments (see Figure 7).

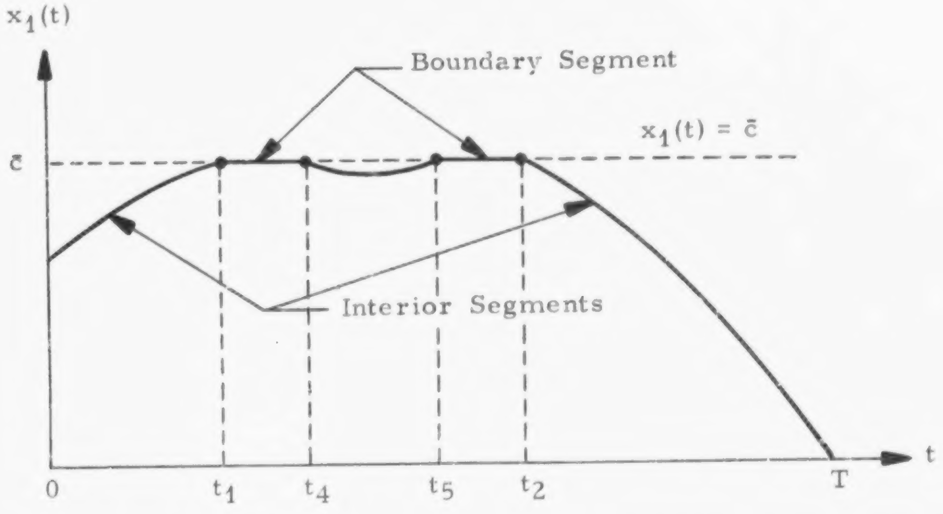


FIGURE 7. A TYPICAL OPTIMAL TRAJECTORY FOR PROBLEM B WITH STATE VARIABLE CONSTRAINT

The nature of the boundary segments in Problem B can be determined by the state variable constraint (4-25) and hence $x_1(t) \equiv \bar{c}$ for all $t \in [t_1, t_2] \subset [0\ ,\ T]$, in which $[t_1, t_2]$ is a boundary segment. It is possible that $[t_1, t_2]$ degenerates to a single point.

It may also be noted that in the sense of Bryson, Denham, and Dreyfus [21] the state constraint (4-25) is a second-order state-variable inequality constraint. Hence (4.20) b. with $k = 1, 2$ determines optimal $u(t)$ when the solution is on the constraint boundary.

$$\left.\begin{aligned} x_1(t) &= \bar{c} \\ -x_0(t) &= \frac{a(t)}{b(t)}\,\bar{c} - F = Q(t)\bar{c} - F \\ u(t) &= u^b(t) = \bar{c}\,\frac{a(t)}{b(t)}\left\{\frac{1}{a}\frac{da}{dt} - \frac{1}{b}\frac{db}{dt}\right\} \\ &= \bar{c}\,\frac{dQ(t)}{dt} \text{ where } Q(t) = \frac{a(t)}{b(t)} \end{aligned}\right\} \begin{array}{l}\text{for all } t \in [t_1, t_2] \subset \\ [0\ ,\ T] \text{ where } [t_1, t_2] \\ \text{is a boundary segment.}\end{array} \tag{4-38}$$

As $u(t)$ also has to satisfy (4-26), the condition (4-39) must hold for all $t \in [t_1, t_2]$.

$$0 \leqq \underline{u} \leqq \frac{a(t)}{b(t)}\,\bar{c}\left(\frac{1}{a}\frac{da}{dt} - \frac{1}{b}\frac{db}{dt}\right) = \bar{c}\,\frac{dQ}{dt} \leqq \bar{u} \ . \tag{4-39}$$

Hence, the optimal trajectory cannot have a boundary segment of positive duration with $x_1^*(t) = \bar{c}$ in any interval $[t_1, t_2] \subset [0\ ,\ T]$ where $dQ/dt < 0$ though it may touch the boundary at isolated points. If $a(t)$ and $b(t)$ remain constant with t , $dQ/dt = 0$ and if $\underline{u} \neq 0$, there is no boundary segment of positive duration; if $\underline{u} = 0$, we may have a boundary segment with $u^*(t) = 0$.

Physically, (4-38) may be considered as expressing the capacity of the channel for waste transport to be $Q(t)\bar{c}$, the product of volume flow rate and maximum allowable concentration. An amount F of this capacity has been used upstream of the origin.

No boundary segment with $x_1^*(t) \equiv 0$ is feasible, because using (4.20) b. to this constraint, $x_1^*(t) = 0$; but $x_0(t) = -\int_0^t u(y)dy$ is a decreasing function of t and $x_0(0) = 0$.

An optimal trajectory to this problem must touch the boundary $x_1(t) = \bar{c}$ in at least one point. The nature of the interior segments, the values of t at which the optimal trajectory touches the boundary for the first time and for the last time and the nature of the trajectory in between these two values of t , may be determined as follows:

The Initial Segment of the Optimal Trajectory

Assume t_1 is the value of t at which the optimal trajectory enters the boundary for the first time. The initial and terminal conditions for this segment are given, using Theorem (4.20) b., as

$$x_0(0) = 0 \text{ and } x_0(t_1) = F - \frac{a(t_1)}{b(t_1)}\,\bar{c}\ ,\ x_1(t_1) = \bar{c}\ . \tag{4-40}$$

The solution of the adjoint system is given by (4-30) for all $t \in [0\ ,\ t_1]$. The transversality conditions at the initial point and the condition $\pi_0(t_1) \geqq 0$ gives (4-32) for all $t \in [0\ ,\ t_1]$. The optimal value of the control variable is given by using Theorem (4.16) as $u^*(t) \equiv \bar{u}\ \forall\ t \in [0\ ,\ t_1]$.

The optimal trajectory is given by $x_0^*(t) = -\bar{u}t$ and

$$x_1^*(t)e^{-\int_0^t a(y)dy} = \omega_2 - \int_0^t \left[b(s)(\bar{u}s + F)e^{-\int_0^s a(y)dy} \right] ds, \; t \in [0\, , t_1] \qquad (4\text{-}35)$$

where ω_2 is given by the terminal condition $x_1(t_1) = \bar{c}$

$$\omega_2 = \bar{c}e^{-\int_0^{t_1} a(y)dy} + \int_0^{t_1} \left[b(s)(\bar{u}s + F)e^{-\int_0^s a(y)dy} \right] ds \; . \qquad (4\text{-}41)$$

The as yet unknown value of t_1 is the least $t_1 > 0$ for which

$$x_0^*(t_1) = -\bar{u}t_1 = F - \frac{a(t_1)}{b(t_1)}\bar{c} \text{ is satisfied.} \qquad (4\text{-}42)$$

For the Constant Coefficient Case (A1, Table I) the results are

$$x_1^*(t) = \frac{b}{a}\left\{\bar{u}\left(t + \frac{1}{a}\right) + F\right\} - \frac{b}{a}e^{a(t-t_1)}\left\{\bar{u}\left(t_1 + \frac{1}{a}\right) + F\right\}$$

$$- \bar{c}e^{a(t-t_1)} \quad \text{for } t \in [0\, , t_1] \text{ and}$$

$$x_1^*(0) = \frac{b}{a}\left\{\frac{\bar{u}}{a} + F\right\} - \frac{b}{a}\left\{\bar{u}\left(t_1 + \frac{1}{a}\right) + F\right\}e^{-at_1} - \bar{c}e^{-at_1} \qquad (4\text{-}43)$$

$$x_0^*(t_1) = F - \frac{a}{b}\bar{c} \text{ and}$$

$$t_1 = \frac{1}{u}\left[\frac{a\bar{c}}{b} - F\right] .$$

The Final Segment of the Optimal Trajectory

Assume t_2 to be the value of t at which the optimal trajectory leaves the boundary for the last time. Evidently $t_1 \leqq t_2 < T$. This interior segment must satisfy Theorm (4.16) and the terminal conditions are given by

$$x_1(t_2) = \bar{c} \text{ and } x_1(T) = 0 \; . \qquad (4\text{-}44)$$

The adjoint variables are again given by (4-30). The minimum principle of Theorem (4.16) is given here by

$$-\pi_0(t)u^*(t) = \min_{u(t)\epsilon P(t)} [-\pi_0(t)u(t)] \qquad (4\text{-}45)$$

for almost all $t \in [t_2, T]$ and therefore

$$\pi_0(t) \geqq 0 \; .$$

Hence the optimal value of the control variable is

$$u^*(t) \equiv \bar{u} \;\forall\; t \in [t_2, T]$$

and the optimal trajectory during $[t_2, T]$ is obtained by substitution into the state equations and integration:

$$x_0^*(t) = x_0^*(t_2) - \bar{u}(t - t_2) \ \forall \ t \in [t_2, T] \tag{4-46}$$

$$\frac{dx_1^*(t)}{dt} = a(t)x_1^*(t) + b(t)[x_0^*(t_2) + \bar{u}t_2 - F - \bar{u}t] \ . \tag{4-47}$$

Integrating,

$$x_1^*(t)e^{-\int_{t_2}^{t} a(y)dy} = \omega_3 - \int_{t_2}^{t} \left[b(s)\{\bar{u}s + F - x_0^*(t_2) - \bar{u}t_2\}e^{-\int_0^s a(y)dy} \right] ds$$

$$\text{for all} \quad t \in [t_2, T] \ . \tag{4-48}$$

The constant ω_3 is given by the boundary condition $x_1(T) = 0$. From (4-47), $dx_1^*(t)/dt = 0$ at $t = t_2$; i.e., the optimal trajectory is tangential to the boundary while leaving at t_2 . The same is true for the initial interior segment at the point of entry t_1 . The value of t_2 is yet unknown and this could be obtained from (4-48) and the initial condition $x_1^*(t_2) = \bar{c}$ by analytic or numerical means. Knowing t_2 , one finally obtains

$$x_0^*(T) = x_0^*(t_2) - \bar{u}(T - t_2) \tag{4-49}$$

where $-x_0^*(T)$ represents the maximum amount of total discharge rate of the constituent into the receiving waters without violating the given quality standard.

The Nature of the Optimal Trajectory During $[t_1, t_2]$

The nature of the optimal trajectory during $[t_1, t_2]$ is basically determined by $Q(t)$, the volume flow rate at a section of the estuary. The important questions to be answered are whether the optimal trajectory remains on the boundary during the whole period $[t_1, t_2]$ or it leaves the boundary to return later and, if so, where are the junction points between the boundary and interior segments.

The optimal trajectory enters the boundary tangentially at t_1 with $u^*(t_1-) = \bar{u}$ and if (4-39) is satisfied by $u^b(t_1)$ obtained in (4-38) from the condition given in Theorem (4.20) b., it continues along the boundary to t_2, if (4-39) is not violated during $[t_1, t_2]$, with the optimal control $u^*(t) = u^b(t)$ during this period. If $u^b(t_1) < \underline{u}$, the optimal trajectory leaves the boundary tangentially touching it at a single point t_1 and the optimal control is switched to $u^*(t_1+) = \underline{u}$.

For the interior segment of the trajectory,

$$x_0^*(t) = x_0^*(t_1) - \underline{u}(t - t_1)$$

$$\frac{dx_1^*(t)}{dt} = a(t)x_1^*(t) + b(t)[x_0^*(t_1) - \underline{u}(t - t_1) - F] \tag{4-50}$$

$$x_1^*(t)e^{-\int_{t_1}^{t} a(y)dy} = \omega_4 - \int_{t_1}^{t} \left[b(s)\{\underline{u}s + F - x_0^*(t_1) - \underline{u}\,t_1\}e^{-\int_0^s a(y)dy} \right] ds$$

for all $t \in [t_1, t_3]$ where it is supposed that the trajectory returns to the boundary at $t_3 \leqq t_2$. However, if $\bar{c}dQ/dt < \underline{u}$ for all $t \in [t_1, t_2]$, $u^b(t) < \underline{u}$ and $t_3 = t_2$; the optimal trajectory touches the boundary at t_2 and the optimal control is switched from $u^*(t_2-) = \underline{u}$ to $u^*(t_2+) = \bar{u}$. In this case

$$x_0^*(T) = -\bar{u}(t_1 + T - t_2) - \underline{u}(t_2 - t_1) \ . \tag{4-51}$$

But if t_3 is the smallest value such that $\bar{c}\, dQ/dt \geq \underline{u}$ for $t \geq t_3$, the optimal trajectory returns to the boundary at t_3 and the optimal control $u^*(t_3-) = u^*(t_3+) = u^b(t_3)$ due to the continuity of $Q(t)$. For the remaining interval $[t_3, t_2]$ the trajectory will be on the boundary with $u^*(t) = u^b(t)$ if (4-39) is satisfied.

Similarly, if $u^b(t) \geq \bar{u}$ for some $t \in [t_1, t_2]$ and t_4 is the smallest value of t for which this happens the optimal trajectory will leave the boundary at t_4 and the control function will change to $u^*(t) = \bar{u}$ for $t \in [t_4, t_5]$ where $t_5 < t_2$ is the point at which it returns to the boundary. Again due to continuity of $Q(t)$, $u^*(t_4-) = u^*(t_4+) = u^b(t_4) = \bar{u}$.

Then for this interior segment of the trajectory

$$x_0^*(t) = x_0^*(t_4) - \underline{u}(t - t_4) = F - \frac{a(t_4)}{b(t_4)}\bar{c} - \underline{u}(t - t_4) \qquad (4\text{-}52)$$

$x_1^*(t)$ is easily obtained from the state equations.

The same reasoning will hold for the rest of the interval $[t_5, t_2]$. Thus knowing the function $Q(t)$ the nature of the optimal trajectory during $[t_1, t_2]$ could be ascertained. It may consist of the following three types of segments (see Figure 7):

a. Boundary segment with $u^*(t) = u^b(t)$, $x_0^*(t) = F - \frac{a(t)}{b(t)}\bar{c}$, $x_1^*(t) = \bar{c}$.

b. Interior segment with $u^*(t) = \underline{u}$, $x_1^*(t) < \bar{c}$.

c. Interior segment with $u^*(t) = \bar{u}$, $x_1^*(t) < \bar{c}$.

While moving along the boundary segment if $u^b(t)$ violates (4-39) either segment b. or c. is obtained, depending on whether it violates the left or right inequality (see Figure 8).

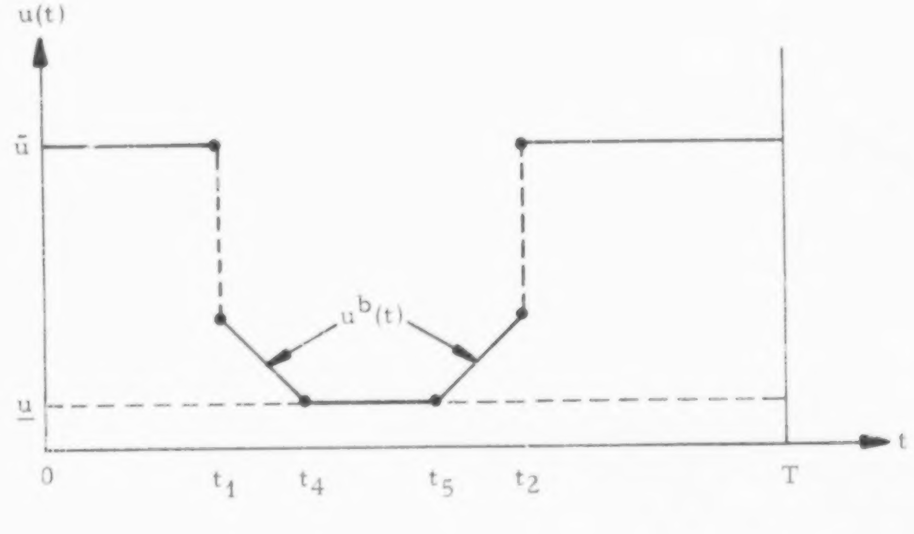


FIGURE 8. THE OPTIMUM CONTROL FUNCTION FOR THE TRAJECTORY IN FIGURE 7

Some Special Variable Coefficient Cases

The solutions for various special forms of the functions $a(t)$ and $b(t)$ described in Table I of Chapter II is presented in Table II. Closed form expressions are often difficult to obtain for the variable coefficient cases. The cases of Table I mainly differ in what happens to the optimal trajectory during $[t_1, t_2]$. It is seen that $dQ(t)/dt$ is the critical quantity when the trajectory is on the boundary and the behavior of the optimal trajectory, and the value of the optimal control depends on relative values of $\bar{c}$, $\underline{u}$, and $\bar{u}$. If $\bar{c}dQ(t)/dt < \underline{u}$, $u^*(t)$ is constrained at $\underline{u}$ and the trajectory leaves the boundary; otherwise $u^*(\bar{t})$ will increase with increasing $\bar{c}dQ(t)/dt$ until it reaches $\bar{u}$, at which time the trajectory will leave the boundary again with $u^*(t) = \bar{u}$.

Problem C

In Chapter II, Problem C has been expressed by (2-22) through (2-25). Consider a special case of this model where $h(c(x))$ and $\ell(S(x))$ are linear and are given by

$$h(c(x)) = h_1c^1(x) + h_2c^2(x) + \dots + h_Mc^M(x) \quad \text{and} \tag{4-53}$$

$$\ell(S(x)) = \ell_1S^1(x) + \ell_2S^2(x) + \dots + \ell_MS^M(x) \ . \tag{4-54}$$

The following substitutions are made to express this problem as a standard linear optimal control problem.

$$t = x \ , \ T = L \ , \ x_o(t) = \int_o^t h(c(x))dx - \int_o^t \ell(S(x))dx$$

$$\left.\begin{aligned} x_m(t) &= c^m(x) \\ u_m(t) &= S^m(x) \\ F_m &= T_o^m \end{aligned}\right\} \quad m = 1, 2, \dots, M \ .$$

$$y_m(t) = \int_o^t S^m(y)dy \ ; \quad m = 1, 2, \dots, M \ .$$

For simplicity, assume

$$L_S^m(t) = \underline{u}_m \ , \ U_S^m(t) = \bar{u}_m \ \text{ and } \ U_c^m(t) = \bar{c}_m \ \forall \ t \in [0 \ , T] \ , \quad m = 1, 2, \dots, M \ .$$

With these substitutions Problem C now becomes, with $x_i = x_i(t)$, $t \in [0 \ , T]$.

Minimize $x_o(T)$

$$\text{Subject to } \frac{dx_o}{dt} = h_1x_1 + h_2x_2 + \dots + h_Mx_M - (\ell_1u_1 + \ell_2u_2 + \dots + \ell_Mu_M) \tag{4-55}$$

$$\left.\begin{aligned} \frac{dx_i}{dt} &= a(t)x_i - b(t)y_i - b(t)F_i \\ \frac{dy_i}{dt} &= u_i(t) \end{aligned}\right\} \quad i = 1, 2, \dots, M$$

with $x_o(0) = 0$; $y_i(0) = 0$; $x_i(T) = 0$ for all $i = 1, 2, \dots, M$.

TABLE II

SOLUTION OF PROBLEM B UNDER SIMPLIFIED ASSUMPTIONS FOR FLOW RATE $Q(t)$

Case	$Q(t)$	$\frac{dQ(t)}{dt}$	$u^*(t)$ on the Boundary	$-x_o^*(t)$ on the Boundary	Remarks
A	Constant $Q(t) = Q_o$	0	If $\underline{u} = 0$, $u^*(t) = 0$ If $\underline{u} > 0$, no boundary segment	$\frac{a\bar{c}}{b} - F$	If $\underline{u} = 0$, boundary segment (a) during $[t_1,t_2]$
B	Linear $Q(t) = Q_o(1 + qt)$	$Q_o q$	$u^*(t) = \bar{c}Q_o q$ if $\underline{u} \leq \bar{c}Q_o q \leq \bar{u}$	$cQ_o(1 + qt) - F$	Trajectory, once on the boundary do not leave during $[t_1,t_2]$
C	Exponential $Q(t) = Q_o e^{\varepsilon t}$	$\varepsilon Q_o e^{\varepsilon t}$	$u^*(t) = \bar{c}\varepsilon Q_o e^{\varepsilon t}$ if $\underline{u} \leq \bar{c}\varepsilon Q_o e^{\varepsilon t} \leq \bar{u}$	$cQ_o e^{\varepsilon t} - F$	Trajectory may leave the boundary 1) at t_1 with segment (b) if $u^b(t_1) < \underline{u}$ and/or 2) at $t_3 < t_2$ if $\bar{c}\varepsilon Q_o e^{\varepsilon t_3} = \bar{u}$
C'	Negative Exponential $Q(t) = Q_o(1 - e^{-\varepsilon t})$	$-\varepsilon Q_o e^{-\varepsilon t}$	No boundary segment possible	——	Trajectory leaves the boundary during $[t_1,t_2]$ with segment (b)

If (4-55) is expressed in the form

$$\text{Minimize} \quad x_o(T)$$

$$\text{Subject to } \frac{dx}{dt} = A(t)x(t) + B(t)u(t) + d(t) \ , \ t \in [0 \ , \ T]$$

then,

$$x = (x_o, x_1, \ldots, x_M, y_1, \ldots, y_M)$$

$$u = (u_1, u_2, \ldots, u_M)$$

$$A(t) = \begin{bmatrix} 0 & h_1 & h_2 & \cdots & h_M & 0 & 0 & \cdots & 0 \\ 0 & a(t) & \cdots & & 0 & -b(t) & & \cdots & 0 \\ \vdots & & a(t) & & \vdots & \vdots & -b(t) & & \vdots \\ 0 & & & \ddots & a(t) & 0 & & \ddots & -b(t) \\ & & \bigcirc & & & & \bigcirc & & \end{bmatrix} \quad d(t) = -b(t) \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_M \\ \vdots \\ 0 \end{bmatrix}$$

$$B(t) = \begin{bmatrix} -\ell_1 & -\ell_2 & \cdots & -\ell_M \\ 0 & & & 0 \\ \vdots & & \cdots & \vdots \\ 0 & & & 0 \\ 1 & & \cdots & 0 \\ & 1 & \ddots & \\ 0 & & \cdots & 1 \end{bmatrix} .$$

The adjoint system $d\pi/dt = -\pi A(t)$ is described by the following set of differential equations, where π is a $(2M + 1)$ vector, and $\pi_i = \pi_i(t)$.

$$\begin{aligned} \frac{d\pi_o}{dt} &= 0 \\ \frac{d\pi_i}{dt} &= h_i\pi_o + a(t)\pi_i \ ; \quad i = 1, 2, \ldots, M \qquad (4\text{-}56) \\ \frac{d\pi_{M+i}}{dt} &= -b(t)\pi_i \ ; \qquad i = 1, 2, \ldots, M \ . \end{aligned}$$

Solution of the above equations gives

$$\pi_o = k_o \text{ (constant)} \quad \text{and} \quad k_o \geq 0 \qquad (4\text{-}57)$$

from Theorem (4.16).

$$\pi_i e^{-\int_o^t a(y)dy} = k_{1i} + \int_o^t \left[k_o h_i e^{-\int_o^s a(y)dy} \right] ds \qquad (4\text{-}58)$$

where k_{1i} is constant and $i = 1, 2, \ldots, M$.

$$\pi_{M+i} = k_{2i} - \int_o^t b(t)\pi_i \qquad (4\text{-}59)$$

where k_{2i} is a constant and $i = 1, 2, \ldots, M$.

For the constant coefficient case (Al, Table I), we have $a(t) \equiv a$, $b(t) \equiv b \ \forall \ t \in [0 , T]$ and from above,

$$\pi_i = k_{1i}e^{at} - k_o \frac{h_i}{a} ; \quad i = 1, 2, \ldots, M \ \text{ and} \qquad (4\text{-}58a)$$

$$\pi_{M+i} = k_{2i} - \frac{k_{1i}b}{a} e^{at} + \frac{k_o h_i t}{a} . \qquad (4\text{-}59a)$$

Using Theorem (4.16) and considering $u^*(t)$ as the optimal control,

$$\pi(t)B(t)u^*(t) = \min_{u(t)\epsilon P(t)} [\pi(t)B(t)u(t)] .$$

According to this condition $u^*(t)$ must minimize for almost all $t \in [0 , T]$ the expression

$$\sum_{i=1}^{M} u_i \left[-k_o \ell_i + k_{2i} - k_{1i} \frac{b}{a} e^{at} + k_o \frac{h_i t}{a} \right] \qquad (4\text{-}60)$$

for all $u(t) \in P(t)$. The next step is to apply the transversality condition as given in Theorem (4.18) at the initial point, where

$$X^o = \{x \mid x_o = 0 , y_i = 0 , i = 1, \ldots, M\} .$$

This gives

$$[\pi_o(0), \pi_1(0), \ldots, \pi_M(0), \pi_{M+1}(0), \ldots, \pi_{2M}(0)] \begin{bmatrix} 0 \\ x_1(0) - x_1^*(0) \\ \cdot \\ \cdot \\ \cdot \\ x_M(0) - x_M^*(0) \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \geqq 0$$

for all $x(0) \in X^o$ or

$$\sum_{i=1}^{M} \pi_i(0)[x_i(0) - x_i^*(0)] \geqq 0 . \qquad (4\text{-}61)$$

This holds for all $x(0) \in X^o$ only if $\pi_i(0) = 0 \ \forall \ i = 1, \ldots, M$. Hence,

$$k_{1i} = \frac{k_o h_i}{a} , \quad i = 1, 2, \ldots, M \qquad (4\text{-}62)$$

and (4-60) reduces to

$$\sum_{i=1}^{M} u_i \left[k_o \left\{ \frac{h_i}{a} \left(t - \frac{b}{a} e^{at} \right) - \ell_i \right\} + k_{2i} \right] . \qquad (4\text{-}63)$$

Hence $h_i > 0$, $\ell_i > 0 \;\forall\; i$, and $k_o \geqq 0$; and the optimal control is given by

a. $u_i^*(t) = \underline{u}_i$ if $R_i(t) = k_o \left\{ \frac{h_i}{a} \left(t - \frac{b}{a} e^{at} \right) - \ell_i \right\} + k_{2i} > 0$ and

b. $u_i^*(t) = \bar{u}_i$ if $R_i(t) = k_o \left\{ \frac{h_i}{a} \left(t - \frac{b}{a} e^{at} \right) - \ell_i \right\} + k_{2i} < 0$.

It may be noted that $R_i(t)$, the expression within brackets in (4-63), is increasing with increasing t for small values of t; but for larger values of t , $R_i(t)$ may be decreasing with increasing t . At $t = 0$, this expression is given by

$$R_i(0) = R_i^o = k_{2i} - k_o \left[\frac{h_i b}{a^2} + \ell_i \right] .$$

Consider the two alternative possibilities:

1. $R_i^o > 0$. Hence $u_i^*(0+) = \underline{u}_i$. With increasing t , $R_i(t)$ is increasing and if it crosses zero then $u_i^*(t)$ will change to $\bar{u}_i$ and will continue at this value until $t = T$ unless for large values of t , $R_i(t)$ again becomes negative.

2. $R_i^o < 0$. Hence $u_i^*(0+) = \bar{u}_i$. With increasing t , $R_i(t)$ is increasing and, if it crosses zero, $u^*(t)$ will switch to $\underline{u}_i$. There is a possibility of its again being switched back to $\bar{u}_i$ if $R_i(t)$ starts decreasing at larger values of t and crosses zero.

The actual optimal trajectory will depend on the relative values of h_i , ℓ_i , a , b , k_o , and k_{2i} .

V. MATHEMATICAL PROGRAMMING FORMULATION
OF THE DISPERSION MODEL

INTRODUCTION

In the preceding chapter, optimal solutions for several steady state dispersion models, obtained by the application of optimal control theory, have been presented. They provide a very good idea regarding the nature of the optimal control policy for discharging pollutants and the effect of various physical and hydrological factors on the optimal policy. This may be of great benefit while deciding land use and industrial and municipal locations around the estuary. However, for the development and solution of these continuous models, it is necessary to know the analytical nature of the relations expressing the cross-sectional area A, advective velocity v, and dispersion coefficient E as continuous functions of the distance along the estuary. A and v can only be measured at discrete sample sections along the estuary to obtain such functions. Several theoretical expressions have been suggested [7] for estimating the value of the dispersion coefficient E as a function of various hydrological parameters (velocity, hydraulic radius, etc.) but none seem quite satisfactory when compared with the values of E estimated from measured concentration profile in an estuary. This may be due to tidal and other currents and deviations from one-dimensional flow. In any case, the only satisfactory method available to date is the estimation of dispersion coefficients from discrete sampling at several sections along the estuary, and approximation by a continuous function.

It is also not possible to obtain analytical solutions for the diffusion model in closed form unless these functions have simple algebraic forms, whereupon numerical approximations may be needed. From the point of view of implementing these results, it is also necessary to convert the discharge rate function $u^*(t)$ to a discrete function having positive values only at a finite number of points along the estuary inasmuch as only a finite number of outfalls is possible.

From these considerations, it seems wise to obtain discrete formulations of the dispersion models discussed in Chapter IV. As illustrated in the following section, the discrete representation of the steady state models generates linear programs [14] and advantage can be taken of the fast computer routines available for the solution of linear programming problems. The nonsteady state models, which give rise to distributed parameter optimal control problems in the continuous case, are also formulated herein as linear programs under discrete approximation. An alternative approach of representing the steady state models as linear programs by dividing the estuary into small longitudinal sections and using the solution of the diffusion equation in each of them to generate the coefficients for the linear program is likewise hereinafter described.

A DISCRETE STEADY STATE FORMULATION

The continuity of the physical process of dispersion in an estuary may be approximated by numerical integration. The integration process commences with a small landward reach and progresses in the seaward direction with the cumulative addition of finite estuarine segments, as shown in Figure 9. The process increases in accuracy with decreasing lengths of estuarine segments, but they are usually dictated by the location of sampling stations. Interest herein is directed not only to finding a concentration profile, but also to the use of this representation to develop Linear Programming Models of problems A, B, and C.

As illustrated in Figure 9 the estuary is divided into n segments, which are denoted as reaches, by locating n + 1 sampling stations at sections numbering from 0 to the n^{th} section. A_i , E_i , v_i , and c_i denote the cross-sectional area,

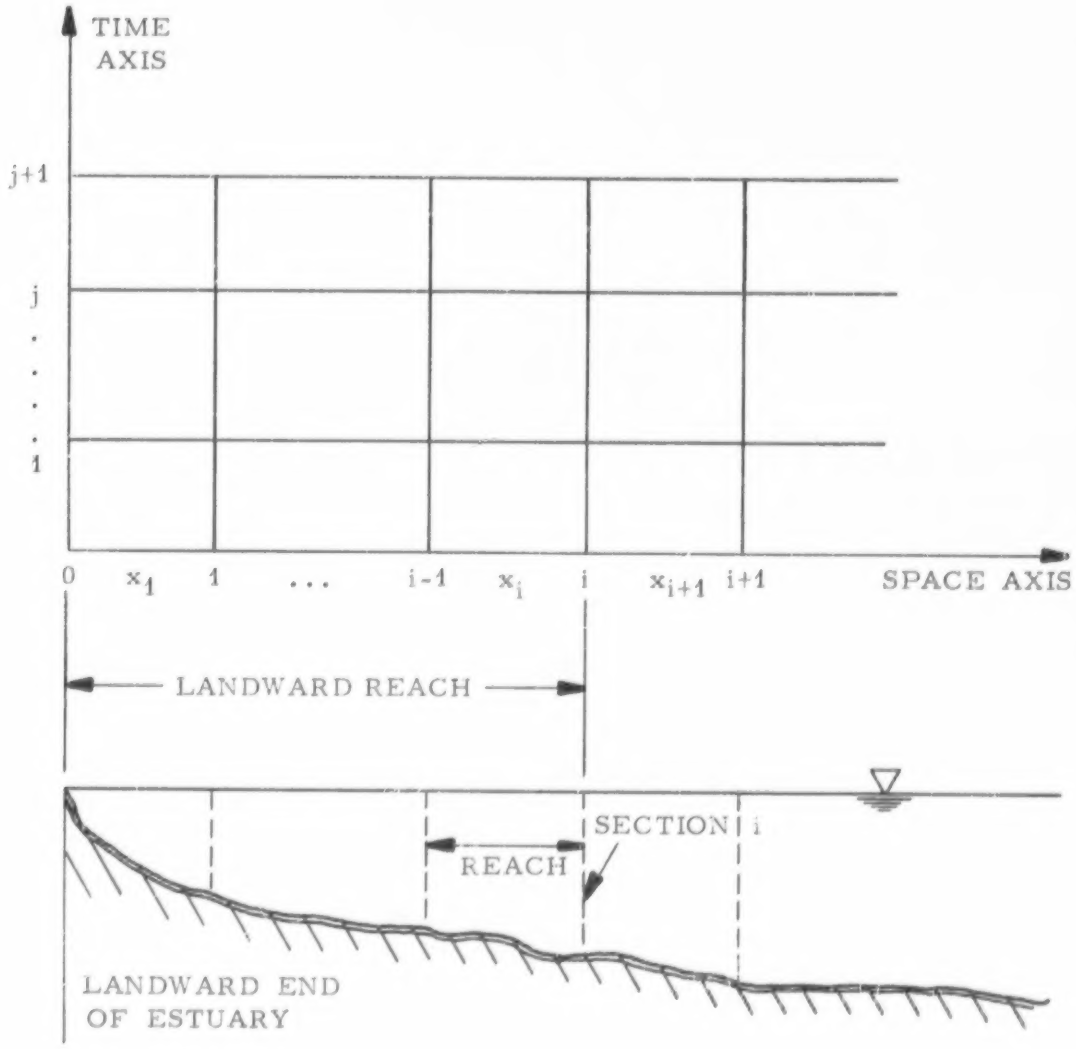

TIME AXIS
j+1
j
1
0
x_1
1
...
i-1
x_i
i
x_{i+1}
i+1
SPACE AXIS
LANDWARD REACH
SECTION i
REACH
LANDWARD END OF ESTUARY

FIGURE 9. FINITE DIFFERENCE SCHEME

dispersion coefficient, advective velocity, and constituent concentration, respectively, at the ith sampling station, whereas S_i denotes the constituent discharge rate per unit time within the i^{th} reach of the estuary. The length of the reaches, x_i, may not be uniform as they depend on convenient locations for sampling stations.

In solving for steady state conservative constituents, Equation (2-10) is the most convenient form to use. It is possible to rewrite Equation (2-10), modified by transport across boundary ($T_o = F$), in terms of central finite differences on the space axis by substituting

$$\left(\frac{dc}{dx}\right)_i = \frac{c_{i+1} - c_{i-1}}{x_{i+1} + x_i} \quad \text{and} \quad c_i = \frac{c_{i+1} + c_{i-1}}{2} .$$

The method of central finite differences has been found [12, 23] to be more accurate and stable than the method of forward differences. Equation (2-10) reduces to

$$A_iE_i\left(\frac{c_{i+1} - c_{i-1}}{x_{i+1} + x_i}\right) = A_iv_i\left(\frac{c_{i+1} + c_{i-1}}{2}\right) - \sum_{k=1}^{i} S_k - F \qquad (5\text{-}1)$$

which may be simplified as

$$c_{i+1} = \frac{2(x_{i+1} + x_i)}{A_i(2E_i - v_i(x_{i+1} + x_i))}\left[\left(\frac{A_iE_i}{x_i + x_{i+1}} + \frac{A_iv_i}{2}\right)c_{i-1} - \sum_{k=1}^{i} S_k - F\right] \qquad (5\text{-}2)$$

and hence

$$c_{i+1} = d_ic_{i-1} - g_i\sum_{k=1}^{i} S_k - g_iF \;; \quad i = 1, 2, \ldots, n-1 \qquad (5\text{-}3)$$

with

$$\left.\begin{aligned} d_i &= g_i\, f_i \\ g_i &= \frac{2(x_i + x_{i+1})}{A_i(2E_i - v_i(x_i + x_{i+1}))} \\ f_i &= A_i\left\{\frac{E_i}{x_i + x_{i+1}} + \frac{v_i}{2}\right\} \end{aligned}\right\} \quad i = 1, 2, \ldots, n-1 \, .$$

From (5-3) are obtained equations expressing c_i as functions of concentrations at other sections and cumulative discharge rate from the landward end to the i^{th} section.

As (5-3) does not involve S_n , an additional equation is obtained by applying (2-10) at the n^{th} section with the approximation

$$\left(\frac{dc}{dx}\right)_n = \frac{c_n - c_{n-1}}{x_n}$$

$$A_nE_n\left(\frac{c_n - c_{n-1}}{x_n}\right) = A_nv_nc_n - \sum_{i=1}^{n} S_i - F \qquad (5\text{-}4)$$

or

$$c_n = \left(\frac{E_n}{E_n - x_nv_n}\right)c_{n-1} - \frac{x_n}{A_n(E_n - x_nv_n)}\left(\sum_{i=1}^{n} S_i + F\right) .$$

This can be simplified as

$$c_n = d_nc_{n-1} - g_n\sum_{i=1}^{n} S_i - g_n F \qquad (5\text{-}5)$$

in which

$$d_n = \frac{E_n}{E_n - x_nv_n} \quad \text{and} \quad g_n = \frac{x_n}{A_n(E_n - x_nv_n)} \; .$$

Equation (5-5) relates concentrations of two adjacent sections, whereas Equation (5-3) does this for sections two reaches apart. Hence an equation such as (5-5) is necessary to relate all the concentrations. A similar equation may be obtained relating c_o and c_1 but its simultaneous use with (5-5) may create redundancy and inconsistency. If S_i are given for all i , then knowing one boundary condition (known value of c_i for any section is sufficient), the concentration profile can be predicted for the whole length of the estuary using (5-3) and (5-5). For more general interest Models A, B, and C can be expressed in discrete forms as follows:

Problem A

Let $\bar{c}$ be the upper bound to the concentration of the constituent under study at any section of the estuary. Equations (5-3) and (5-5) can then be rewritten as the corresponding equations

$$c_{i+1} - d_i c_{i-1} + g_i \sum_{k=1}^{i} S_k + g_i F = 0 \; ; \quad 0 \leqq c_i \leqq \bar{c} \qquad (5\text{-}6)$$

$$i = 1, 2, \ldots, n-1$$

$$0 \leqq c_o \leqq \bar{c}$$

$$c_n - d_n c_{n-1} + g_n \sum_{i=1}^{n} S_i + g_n F = 0 \; ; \quad 0 \leqq c_n \leqq \bar{c} \; . \qquad (5\text{-}7)$$

Now $\bar{c}$, c_i , and S_i may be treated as variables, interrelated through (5-6) and (5-7) and the objective function can be set as

$$\bar{c} = Z \text{ (min)} \; . \qquad (5\text{-}8)$$

S_i are constrained by the relations

$$0 \leqq \underline{S}_i \leqq S_i \leqq \overline{S}_i \; ; \quad i = 1, 2, \ldots, n \qquad (5\text{-}9)$$

due to physical limitations at the outfalls and total discharge quantity $\overline{S}$.

$$S_1 + S_2 + \ldots + S_{n-1} + S_n = \overline{S} \; . \qquad (5\text{-}10)$$

The system consisting of Equations (5-6) through (5-10) constitute a Linear Program [14] and Simplex Method or any modification of it may be used to obtain an optimum solution. However, since no boundary conditions have been imposed on this system, it will not necessarily satisfy any boundary condition that exists in the estuary. Hence, if a boundary condition is known to exist at either the landward or the seaward section which does not change appreciably with changes of S_i (within certain limits), this boundary condition may be imposed on the problem as an added constraint. Such a boundary condition will exist, for example, at a section in the ocean beyond the interface of the estuarine water with the ocean. For purpose of illustration, the boundary condition

$$c_n = b_n \qquad (5\text{-}11)$$

is imposed in which b_n is a given constant ($b_n = 0$ is assumed in Chapter II) though a boundary condition could have been imposed on any c_i . The resulting Linear Program is shown in Table III. Computer codes are available for rapid solution of linear programs. In addition to the values of c_i and S_i , the program also gives the values of the dual or shadow prices. These dual prices are interpreted as the marginal costs of changing g_i , F , b_n , or $\overline{S}$ in terms of corresponding changes in $\bar{c}$ and such information is useful.

For every conservative constituent, a similar linear program could be written down. Since it has been assumed that the values of the dispersion coefficient E do not change with the nature of the constituent and A and v are independent of the constituent, the same values for the matrix coefficients obtain in all such linear programs. The only difference will be in the values of initial load F , the total constituent load $\overline{S}$, and the boundary constituent concentration b_n .

TABLE III

LINEAR PROGRAMMING TABLEAU FOR PROBLEM A

c_0	c_1	c_2	$\cdots$	c_{n-2}	c_{n-1}	c_n	$\bar{c}$	S_1	S_2	$\cdots$	S_{n-2}	S_{n-1}	S_n	RHS
$-d_1$		1						g_1						$= - g_1F$
	$-d_2$		1	.				g_2	g_2					$= - g_2F$
		.	.		.	.								
				$-d_{n-1}$		1		g_{n-1}	g_{n-1}	$\cdots$	g_{n-1}	g_{n-1}		$= - g_{n-1}F$
					$-d_n$	1		g_n	g_n	$\cdots$	g_n	g_n	g_n	$= - g_nF$
1							-1							$= 0$
	1						-1							$= 0$
		.					.							
		.					.							.
			.				.							.
				.			.							.
					.		.							
					.		.							
						1	-1							$= 0$
								1	1		1	1	1	$= \bar{S}$
							1							$= Z(\min)$.

$c_i \geq 0 \quad \underline{S}_i \leq S_i \leq \bar{S}_i \quad \bar{c} \geq 0$.

Due to these advantages, the linear program will be solved for only one conservative constituent, and from its solution, the solution for other constituents could be easily obtained, by multiple right-hand side or parametric programming approach [24]. A modification of the pertinent equations to include the decay terms will again lead to a linear program for nonconservative constituents. (Cf. Appendix A.) In this form, the effects of changing the linear reaction coefficients may also be studied.

Problem B

Assume U_i to be the allowable maximum concentration of a constituent at the i^{th} section of the estuary. Then Equations (5-3) and (5-5) can again be rewritten

$$c_{i+1} - d_i c_{i-1} + g_i \sum_{k=1}^{i} S_k + g_i F = 0 \; ; \quad 0 \leq c_i \leq U_i \qquad (5\text{-}12)$$

$$i = 1, 2, \ldots, n-1$$

along with $0 \leq c_0 \leq U_0$ and

$$c_n - d_n c_{n-1} + g_n \sum_{k=1}^{n} S_k + g_n F = 0 \; ; \quad 0 \leq c_n \leq U_n \; . \qquad (5\text{-}13)$$

Usually, $U_i \equiv U \; \forall \; i$, i.e., the same upper bound will be used throughout the estuary, but if desired, different values may be imposed depending on the use of the water body or other considerations.

Now c_i and S_i may be treated as variables interrelated through the Equations (5-12) and (5-13) and the objective function can be set as

$$\text{Maximize } D = S_1 + S_2 + \ldots + S_n \qquad (5\text{-}14)$$

where S_i are again constrained by physical limitations at the outfalls.

$$0 \leq \underline{S}_i \leq S_i \leq \overline{S}_i \; ; \quad i = 1, 2, \ldots, n \; . \qquad (5\text{-}15)$$

The system consisting of Equations (5-12) through (5-15) constitute a linear program and as in Problem A, a boundary condition may be imposed.

$$c_n = b_n \leq U_n \; . \qquad (5\text{-}17)$$

The resulting linear program is shown in Table IV. The same remarks regarding the conservative and nonconservative constituents following Problem A are applicable in this case also. The solution obtained using available computer programs gives the optimal values of c_i , S_i and the dual shadow prices. The dual shadow prices are interpreted as the marginal costs of changing U_i expressed in terms of the corresponding changes in maximum value of D . For different conservative components, only the right-hand side of the linear program will change. So a standard linear program code with multiple right-hand side facility may be used to obtain solutions for all conservative components. A parametric programming approach [24] may be used to study the effects of changing the water quality standards U_i , $i = 0, 1, 2, \ldots, n$.

Problem C

If linear (convex) cost functions are assumed to represent $h(c(x))$ and $\ell(S(x))$ in Model C, by a similar process of discretization, it may be expressed as a linear (convex) programming problem.

The inequalities (5-12) and (5-13) may be modified to cover all effluent components, the superscripts indicating the component.

TABLE IV

LINEAR PROGRAMMING TABLEAU FOR PROBLEM B

c_o	c_1	c_2	$\cdots$	c_{n-2}	c_{n-1}	c_n	S_1	S_2	S_3	$\cdots$	S_{n-2}	S_{n-1}	S_n	RHS
$-d_1$		1					g_1							$= - g_1F$
	$-d_2$.		1				g_2	g_2						$= - g_2F$
		.	.	.										
				$-d_{n-1}$		1	g_{n-1}	g_{n-1}	g_{n-1}	$\cdots$	g_{n-1}	g_{n-1}		$= - g_{n-1}F$
					$-d_n$	1	g_n	g_n	g_n	$\cdots$	g_n	g_n	g_n	$= - g_nF$
							1	1	1	$\cdots$	1	1	1	$= D(\max)$.

$\bar{c} \geqq c_i \geqq 0 \quad i = 0 , 1 , \ldots , n \quad \underline{S}_i \leqq S_i \leqq \bar{S}_i \quad i = 1 , 2 , \ldots , n$.

$$c_{i+1}^m - d_i c_{i-1}^m + g_i \sum_{k=1}^{i} S_k^m + g_i F^m = 0 \; ; \quad 0 \leq c_i^m \leq U_i^m \qquad (5\text{-}18)$$

$$i = 1, 2, \ldots, n-1$$

along with $0 \leq c_o^m \leq U_c^m$ and

$$c_n^m - d_n c_{n-1}^m - g_n \sum_{k=1}^{n} S_k^m - g_n F^m = 0 \; ; \quad 0 \leq c_n^m \leq U_n^m \qquad (5\text{-}19)$$

for $m = 1, 2, \ldots, M$.

Usually $U_i^m \equiv U^m \; \forall \; i , m$; i.e., the same standard may be used at all sections of the estuary for a particular effluent component.

Linear cost functions may be assumed for each section which are additive to give the objective function expressing the total cost along the estuary as

$$\text{Minimize} \quad TC = \sum_{i=o}^{n} \sum_{m=1}^{M} h_i^m c_i^m - \sum_{j=1}^{n} \sum_{m=1}^{M} \ell_j^m S_j^m \qquad (5\text{-}20)$$

where h_i^m and ℓ_i^m are estimated constants. Development of such constants h_i^m for social cost function is described on page 70.

A boundary condition at the ocean end may be described by

$$c_n^m = b_n^m \leq U_n^m \qquad (5\text{-}21)$$

where b_n^m is a constant vector.

The linear program described by (5-18) through (5-21) is a large-sized program, the matrix A consisting of M(n+1) rows and M(2n+1) columns with M(n+1) upper bounded variables when expressed in the form $Ax = b$. For $M = 10$, and $n = 50$, it generates a 510 x 1010 matrix with 510 upper bounded variables. Fortunately, however, the coefficient matrix has a block angular structure (Table V) consisting of similar diagonal submatrices, A_m , $m = 1, 2, \ldots, M$, with each A_m the same as the coefficient matrix in Table IV. Due to this regular structure, essentially there are M comparatively small linear programs each of the size of the basic block which are tied together to give the linear program for Problem C.

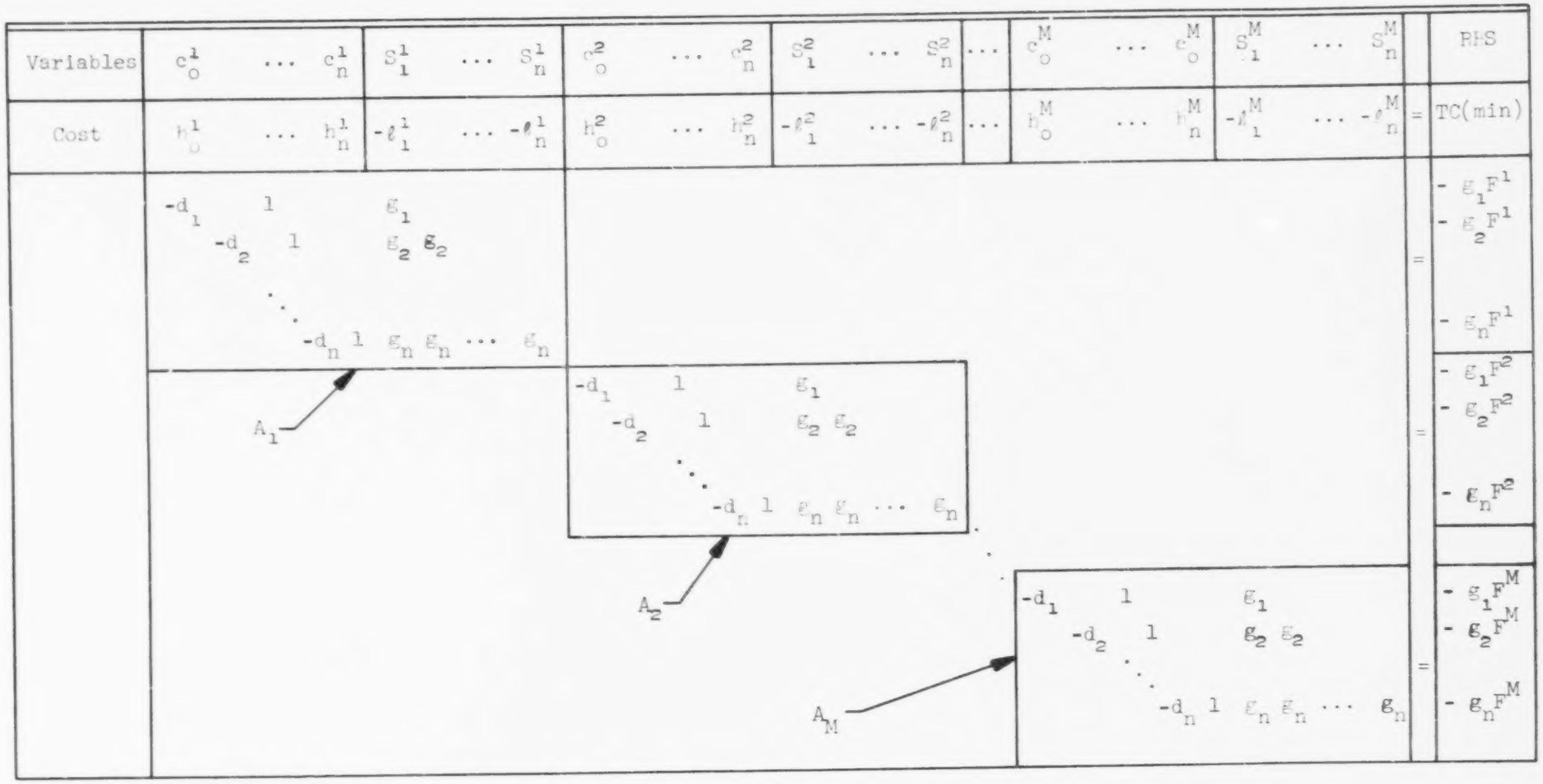
It is obvious that the large linear program could be split up into M smaller subproblems, one for each component represented by a block and the corresponding objective equation. These smaller linear programs (51 x 101 with data of the last section) could be separately solved and optimal values of the objective functions added together to give Min TC . The smaller subproblems are easier to handle with existing codes, and considerable savings in the total computation time is also obtained following this method.

AN ALTERNATIVE DISCRETE STEADY STATE FORMULATION

The numerical method on which the Linear Programming Formulations of problems A and B is based in the preceding section generates a set of linear difference equations, (5-3) and (5-5), relating the concentrations of alternate sections and a linear interpolation scheme (equations (5-1) and (5-4)) is used to approximate the

TABLE V

LINEAR PROGRAMMING FORMULATION FOR MODEL C



Variables	$c^1_o \;\cdots\; c^1_n$	$S^1_1 \;\cdots\; S^1_n$	$c^2_o \;\cdots\; c^2_n$	$S^2_1 \;\cdots\; S^2_n$	$\cdots$	$c^M_o \;\cdots\; c^M_o$	$S^M_1 \;\cdots\; S^M_n$		RHS
Cost	$h^1_o \;\cdots\; h^1_n$	$-\ell^1_1 \;\cdots\; -\ell^1_n$	$h^2_o \;\cdots\; h^2_n$	$-\ell^2_1 \;\cdots\; -\ell^2_n$	$\cdots$	$h^M_o \;\cdots\; h^M_n$	$-\ell^M_1 \;\cdots\; -\ell^M_n$	=	TC(min)
	$-d_1 \;\; 1$	g_1						=	$-g_1F^1$
	$-d_2 \;\; 1$	$g_2 \;\; g_2$							$-g_2F^1$
	$\ddots$								
	$-d_n \;\; 1$	$g_n \;\; g_n \;\cdots\; g_n$							$-g_nF^1$
			$-d_1 \;\; 1$	g_1				=	$-g_1F^2$
			$-d_2 \;\; 1$	$g_2 \;\; g_2$					$-g_2F^2$
			$\ddots$						
			$-d_n \;\; 1$	$g_n \;\; g_n \;\cdots\; g_n$					$-g_nF^2$
					$\ddots$				
						$-d_1 \;\; 1$	g_1	=	$-g_1F^M$
						$-d_2 \;\; 1$	$g_2 \;\; g_2$		$-g_2F^M$
						$\ddots$			
						$-d_n \;\; 1$	$g_n \;\; g_n \;\cdots\; g_n$		$-g_nF^M$

concentration at the middle section. This process increases in accuracy with decreasing lengths of estuarine segments as shown by Cullum [25]. The lengths of sections are dictated by the location of the sampling stations and these could not be reduced too much due to prohibitive costs. It may be possible to obtain higher accuracy by using a closed form of solution within each section of the estuary. Selleck et al. [12, 26] describe such a method. In this section, the desire is to show that using their representation problems A and B can again be formulated as linear programs under certain simple assumptions.

If all the coefficients (A , E , v) in Equation (2-4) are constants, the concentration term is completely steady from one tidal cycle to the next, the sink term Q_L in S is composed strictly of sinks which are directly proportional to the concentration c existing in the receiving water, and k represents a first-order rate of constituent decay (k = 0 for conservative constituents). Equation (2-4) reduces to

$$E \frac{d^2 c}{dx^2} - v \frac{dc}{dx} - \left(k + \frac{Q_L}{V} \right) c = 0 \qquad (5\text{-}22)$$

where Q_L is the sink flow within the region of concern and V , the total water volume lying in the region.

Equation (5-22) can be integrated directly to give

$$c(x) = e^{\alpha x} \left[c_o \cosh \ \beta x \left(c_o \alpha - \frac{T_o}{AE} \right) \sinh \ \beta x \right] \qquad (5\text{-}23)$$

where $\alpha = \frac{V}{2E}$, and

$$\beta = \alpha \sqrt{1 + \frac{4(k + Q_L/V)E}{v^2}} \ .$$

c(x) is the concentration at x and the boundary conditions are:

c_o = the constituent concentration at x = 0

T_o = the net transport of the constituent mass at x = 0 .

If the estuary is divided into sections of sufficiently small length so that the coefficients of the diffusion equation are approximately constant throughout each section, Equation (5-23) can be used to express the conditions within each section with the average magnitude of coefficients being varied from section to section. The following procedure may be employed for steady state numerical integration. Beginning with an estuarine section having known boundary conditions, the concentration and transport of the constituent at the opposite boundary are computed using equations (5-23) and (2-7). These values in turn are used as known quantities at the boundary of the contiguous section, and the computational process is repeated. In this way a profile of the constituent concentration can be computed for the entire reach.

At cross sections where external sources (wastewater discharges) are contributing masses of the constituent of interest, additional boundary conditions are established by the following considerations:

$$(Q_s c_s)_i = T_i(1) + T_i(2) \qquad (5\text{-}24)$$

where $T_i(1)$ and $T_i(2)$ are the net transport of source mass in the landward and seaward directions, respectively, and $(Q_s c_s)_i$ is the source strength of concentration c_s , all taken at the i^{th} sectional boundary. Also the concentration profile is continuous at the source. Knowing one additional boundary condition at either end of the reach being integrated, the overall profile resulting from the source flow may be computed by trial and error. A computer program for this method is described in [12].

A series of particular solutions of the diffusion equation may be summed up to give a general solution due to the linear nature of the equation. Hence the concentration profiles resulting from several independent sources may be added up to give the resulting constituent profile when these sources act simultaneously. This property of linearity is made use of in the linear programming formulations of problems A and B in this section.

For a source e_i of unit value at section i , the concentration profile c(x , i) can be found, giving the coefficients a_{ki} , a_{ki} being the ordinate of c(x , i) at section k , due to a unit source e_i at section i . These coefficients may be computed for all i = 1, 2, ..., n , and k = 0, 1, 2, ..., n , in a given estuary using the method described earlier in this section. Now, for a pattern of constituent discharge with sources of strength $S_i = [(Q_s c_s)_i]$ at the i^{th} section, i = 1, 2, ..., n , the resulting concentration can be computed at the k^{th} section as

$$c_k = \sum_{i=1}^{n} a_{ki} S_i \; ; \quad k = 0, 1, 2, \ldots, n \tag{5-25}$$

and one can proceed with the linear programming formulation.

Problem A

If $\bar{c}$ is the upper bound of the concentration profile that is to be minimized and $\overline{S}$ is the total amount of constituent to be discharged, the following linear program must be solved.

$$\begin{aligned}
a_{01}S_1 + a_{02}S_2 + \cdots + a_{0n}S_n - \bar{c} &\leq 0 \\
a_{11}S_1 + a_{12}S_2 + \cdots + a_{1n}S_n - \bar{c} &\leq 0 \\
a_{21}S_1 + a_{22}S_2 + \cdots + a_{2n}S_n - \bar{c} &\leq 0 \\
&\vdots \\
a_{n1}S_1 + a_{n2}S_2 + \cdots + a_{nn}S_n - \bar{c} &\leq 0 \\
S_1 + S_2 + \cdots + S_n &= \overline{S} \\
\bar{c} &= Z(\min) \; .
\end{aligned} \tag{5-26}$$

The values of c_i , i = 0, 1, ..., n are obtained from the optimal value of $\bar{c}$ and the slack variables.

Problem B

If U_i is the given upper bound of the concentration at section i which could not be violated and D is the total amount of the constituent that could be discharged, and the desire is to maximize D , the following linear program must be solved.

$$\begin{aligned}
a_{01}S_1 + a_{02}S_2 + \dots + a_{0n}S_n &\leqq U_0 \\
a_{11}S_1 + a_{12}S_2 + \dots + a_{1n}S_n &\leqq U_1 \\
a_{21}S_1 + a_{22}S_2 + \dots + a_{2n}S_n &\leqq U_2 \\
&\;\;\vdots \\
a_{n1}S_1 + a_{n2}S_2 + \dots + a_{nn}S_n &\leqq U_n \\
S_1 + \quad S_2 + \dots + \quad S_n &= D\,(\max)\,.
\end{aligned} \qquad (5\text{-}27)$$

The values of c_i , $i = 0, 1, \dots, n$ are obtained from U_i , $i = 0, 1, \dots, n$ and the values of the slack variables. Again we may set $U_i \equiv U$, $\forall\, i$, if desired.

The solutions of these linear programs give the pattern of discharge that should be followed to attain the desired objectives. As before, the dual or shadow prices, which are marginal costs of changing the right-hand side, are obtained also, both in problems A and B. A similar formulation of Problem C is also possible.

A NONSTEADY STATE MODEL FORMULATION

Any model postulated for a natural estuarine system should include a recognition of long-term nonsteady conditions (even if the usual tidal fluctuations are averaged). Otherwise a steady state model would not succeed in accurately predicting the concentrations of the constituents on an all-year basis. There is always seasonal variations of hydrology with corresponding changes in advective velocity, volume flow and dispersion coefficients, the latter often being a function of the advective velocity. The decay coefficient for degradable substances also seems to change considerably with changes in temperature from summer to winter. Even the verification of a steady state model by actual sampling and investigation becomes difficult because the inputs to most natural estuaries are rarely steady.

A nonsteady state model of dispersion is also desirable in order to permit utilizing the flexibility of changing the pattern and quantity of waste discharges during various seasons (as the production of wastes often have seasonal patterns, e.g., canning industry). Also the effects on water quality of flow augmentation from the reservoirs and/or temporary storage of wastes during periods of low flow could be studied in an integrated model of dispersion and treatment for the whole year.

In this section the development is briefly described of nonsteady state linear programming models for problems A and B from the differential equation (2-4) describing the equilibrium conditions for an effluent component at any section of the estuary. A detailed exposition is carried out in Appendix B.

Letting the subscript 'i' denote the i^{th} section on the longitudinal axis and the subscript 'j' the j^{th} time trace (Figure 9), Equation (2-4) can be written as

$$\left[\frac{\partial}{\partial x}\left(AE\,\frac{\partial c}{\partial x}\right)\right]_{i,j} = \left[\frac{\partial}{\partial x}\,(Avc)\right]_{i,j} + \left[A\,\frac{\partial c}{\partial t}\right]_{i,j} - [S]_{i,j} \qquad (5\text{-}28)$$

It is shown in [23] that employing forward finite-differences the individual terms may be approximated and we finally obtain Equation (44) in [23] reproduced below as

$$c_{i,j+1} = c_{i,j} + \frac{t_{j+1} - t_j}{A_{i,j}}\left[\left(\frac{\partial}{\partial x}\left(AE\,\frac{\partial c}{\partial x}\right)\right)_{i,j} - \left(\frac{\partial}{\partial x}\,(Avc)\right)_{i,j} + (S)_{i,j}\right] \qquad (5\text{-}29)$$

and

$$(S)_{i,j} = (S_s)_{i,j} - (Q_L)_{i,j}c_{i,j} - k_{i,j}A_{i,j}c_{i,j} \tag{5-30}$$

where $(S_s)_{i,j}$ is the source input quantity of the constituent, $(Q_L)_{i,j}$ is the amount of sink withdrawal of water and $k_{i,j}$ is the first-order decay coefficient at section i and time j . It can be shown (Appendix B) that (5-29) is a linear equation involving constants $A_{i,j}$, $E_{i,j}$, $v_{i,j}$, $t_{i,j}$, $x_{i,j}$ and variables $c_{i-1,j}$, $c_{i,j}$, $c_{i+1,j}$, $c_{i,j+1}$, and $S_{i,j}$. It can be expressed as

$$\begin{aligned} c_{i,j+1} &= a_{00}c_{00} + a_{01}c_{01} + \dots + a_{0j}c_{0j} + a_{10}c_{00} + \dots + a_{1j}c_{1j} + \dots \\ &\quad + a_{n1}c_{n1} + \dots + a_{nj}c_{nj} + \Delta_{i,j}(S_s)_{i,j} \end{aligned} \tag{5-31}$$

in which $a_{i,j}$ ($i = 0, 1, \dots, n$, $j = 0, 1, \dots, T$) are known constants most of which are zeros and $\Delta_{i,j} = t_{j+1} - t_j/A_{i,j}$. Now treating $c_{i,j}$'s and $(S_s)_{i,j}$'s as variables, linear programming formulations can be obtained in the sense of problems A or B depending on the desired objective.

Problem A

If no temporary storage of waste is feasible, one may assume

$$(S_s)_j = \sum_{i=1}^{n} (S_s)_{i,j} \equiv L_j \tag{5-32}$$

in which L_j is known, $j = 0, 1, \dots, T$. The linear program is used to minimize $\bar{c}$, the upperbound to the concentration $c_{i,j}$ for all i and all j .

A more interesting case would be when, with certain limitations, lagooning or temporary storage (or production cut) is possible and only

$$\sum_{i=1}^{n} \sum_{j=1}^{M} (S_s)_{i,j} = L \tag{5-33}$$

is specified. With the addition of constraints representing storage limitations to (5-31) and (5-32) or (5-33) a linear program may be formulated to minimize $\bar{c}$.

Problem B

Here it may be assumed that the maximum allowable constituent concentrations $U(i , j)$ have been provided for $i = 0 , 1, \dots, n$, $j = 0, 1, \dots, T$. $c_{i,j}$ and $S_{i,j}$ can be treated as variables and

$$\sum_{i=1}^{n} \sum_{j=1}^{M} S_{i,j} = D \text{ maximized .}$$

If temporary storage or lagooning of effluents is allowed, such provisions can be included in the linear program with appropriate constraints.

Flow augmentation will change the values of $v_{i,j}$ and possibly $A_{i,j}$. Selleck et al. [12] have shown that in the northern San Francisco Bay E varies as $(v)^{3/4}$. Once changes in $v_{i,j}$, $A_{i,j}$, and $E_{i,j}$ are known, new $a_{i,j}$'s may be computed and a sensitivity analysis [14] carried out to study effects of flow augmentation.

DISCUSSION OF DISCRETE MODELS

Problem B formulated either as a steady state or a nonsteady state model (depending on our purpose) forms the first stage of a general two-stage model for water quality control and the plan of discharge obtained as the solution of this problem forms the input to the second stage of the model (to be discussed in the following chapter) which is concerned with finding the optimum plan of treatment of raw effluents.

Problem A is interesting by itself as it indicates an optimum way of discharging a given quantity of waste products. Problem C takes into account the social cost of pollution and the savings in minimum treatment costs associated with the disposal of wastes. It does not provide an optimal plan of treatment as is obtained in the integrated model described in Chapter VII.

It should be emphasized that the two approaches toward discretization presented here are not claimed as the most efficient or accurate ones possible. A method of discretizing continuous optimal control problems similar to the first method is described by Van Slyke [18]. Other finite difference methods such as the Runge-Kutta method are accurate to the order of $(\Delta x)^4$. Harleman, Lee, and Hall used the Stone and Brian method [27] in [28] quite successfully. Most of the numerical methods lead to mathematical programs of the form presented here. Hence the accuracy desired and convenience in using will determine the selection of the most desirable numerical technique.

Appendix C presents a demonstration of the discrete steady state version of Problem B in the Suisun Bay-Lower San Joaquin River area where phosphate has been considered as the steady state constituent to be controlled. Hydrological data collected during "A Comprehensive Study of San Francisco Bay" [12] has been used for this purpose.

The idea of using a linear programming approach for water quality control is not entirely new and has been used by other authors [6, 11, 29, 30]. Thomann and Marks [30] used a transfer function approach to predict the resulting concentration profile in an estuary due to inputs of waste discharges. Their approach is closer in spirit to the alternative discrete steady state formulation described earlier in this chapter, though their method of computation of the transfer function matrix seems complicated. They develop a transfer function matrix for dissolved oxygen and formulate a linear program using this matrix.

In contrast, the models A, B, and C are formulated here as linear optimal control problems and linear programs are generated by a process of discretization. In addition to controlling dissolved oxygen, a better control of various toxic and stable chemicals discharged by industries is needed today. The same linear programs for problems A and B could be used for all conservative constituents with minor changes in the right-hand side and Model C is a multicomponent model. Model B gives an idea for optimal channel capacity of the estuary for waste transport and is useful for deciding and controlling future land use along the estuary.

Deininger [6] and O'Connor [11] both used dissolved oxygen as the quality factor in their work and dispersion was neglected. Their approach is valid for fast flowing rivers. But it cannot adequately represent the complex mixing process in an estuary which includes molecular diffusion, tidal mixing, effects of shear flow, and density stratification.

Development of a dynamic hydraulic water quality model using the network concept for representing two-dimensional effects by a "coarse mesh" of channels and junctions is reported in [31] and recently presented by Orlob et al. [32]. This model is perhaps on its surest ground in representing hydrologic and hydrodynamic behavior of estuarial systems. However, the computational effort needed seems much greater in comparison to the added accuracy obtained in predicting the tidal effects in the estuary. Concentration profiles of salinity and BOD are predicted for given waste loads, but no attempts at optimization are made. Considering the accuracy of the hydrological data available, a one-dimensional representation may be a good one for the time being, though research is needed to develop better representation of the complex mixing process in an estuary.

VI. THE WASTE TREATMENT MODEL

INTRODUCTION

Optimal water quality management in an estuarine basin may be effected in two distinct stages. The first stage consists of optimal allocation of water quality through a study of the dynamics of dispersion and of the self-purifying and assimilative properties of the water basin. This has been described in Chapters II, IV, and V. The subject of this chapter is the second stage which consists of minimizing the sum of treatment costs and social costs due to water pollution (while maintaining acceptable water quality standards in the basin) and utilizing economic growth projections to plan for future treatment capability.

Except in Model C, the treatment and social costs due to pollution has not been considered while formulating the diffusion models. In Model B here, it is implicitly assumed that if the total amount of each of the pollutants discharged are maximized, while maintaining a prescribed standard, the total treatment costs would be minimized over the estuary. The Waste Treatment Model described in this chapter would actually carry out this cost minimization process, using as inputs the optimal discharge plans (generated by a Dispersion Model) along with waste generation and treatment data for the water basin.

The cost of maintaining a prescribed standard is one of the most important factors that should be considered while deciding on such a standard. For an estuarine basin, it is necessary to know the total costs of maintaining a prescribed standard and the marginal costs of changing such standards. Such total costs must include the cost of damages due to pollutional effects and costs of pollution abatement. Damage costs are a function of the quality of the water and should also include any costs of pretreatment necessary to remove pollutional effects from water for domestic or industrial use. Quantitative information is lacking regarding other types of damage costs due to pollutional effects.

In this chapter the aim is to relate a prescribed quality standard of an estuarine region to the corresponding pollution abatement costs incurred by the industrial sectors and municipal bodies of the region who use the estuarine waters for disposal of their waste products. It is possible to maintain the same standard through various means and at varying costs. But we are interested in a plan of action which will minimize the total costs for the whole region. Presumably such a plan may be implemented through a regional organization which would be responsible for allocating the total cost among the waste dischargers in some equitable fashion.

MATHEMATICAL FORMULATION OF THE MODEL [29]

The problem involves a water basin or a part thereof which is used for effluent disposal by various public and private dischargers. It is assumed that the quality of water in the basin is characterized by the amount of certain chemical components such as phenols, BOD, phosphate, nitrogen, etc., which are discharged into the basin in the time period considered and a standard is specified by denoting the maximum amount of each component that could be discharged. Solution of Model B (see Chapter V) for all the relevant components gives such data for each section of the estuary.

The decisions available are the choices of effluent treatment techniques to be used at each of the industrial and municipal units discharging effluents into the basin. These options may range from no treatment through the standard primary, secondary, and tertiary treatments up to the most advanced methods. The optimum (cost-minimizing) decisions are obtained by solving a linear program set up for this purpose. Capital costs for effluent treatment are not considered directly by the model as they give rise to mixed integer programming problems [14] which are difficult to solve.

The waste treatment linear programming model developed by Carew and Van Slyke [29] may be described as follows:

Assume there are L industrial sectors (for example, steel, petroleum, chemical, canning, etc.), and that for each sector ℓ there are K_ℓ possible methods for effluent treatment. The effluent contains M different types of quality characteristics or components such as phenol, chloride, BOD, etc. for which maximum allowable concentrations have been specified (as in Problem B, Chapter II).

The following data are required:

1. $a_{k,\ell,m}$, the amount of effluent component m released per unit of untreated effluent by the k^{th} treatment for industry ℓ ; $k = 1, \ldots, K_\ell$; $\ell = 1, \ldots, L$ and $m = 1, \ldots, M$.

2. b_m , the maximum allowable amount of effluent m totaled over all industries that could be discharged. This could be obtained from the solution of Problem B, Chapter V, for these constituents. Let d_ℓ be the total amount of untreated effluent (of known composition) produced by the industrial sector ℓ .

3. $c_{k,\ell}$, the cost of treating one unit of raw effluent (of known composition) from industry ℓ by treatment k .

The model determines a set of decision variables $x_{k,\ell}$, interpreted as the amount of untreated effluent from sector ℓ to be treated by method k , in such a way that the total cost taken over all industrial sectors is minimized. This formulation leads to the following set of equations:

$$\sum_{\ell=1}^{L} \sum_{k=1}^{K_\ell} a_{k,\ell,m}\, x_{k,\ell} \leqq b_m \;; \qquad m = 1, \ldots, M \tag{6-1}$$

meaning that the total amount of effluent component m left after treatment should not exceed the specified maximum allowable amount b_m to be discharged.

$$\sum_{k=1}^{K_\ell} x_{k,\ell} = d_\ell \;; \qquad \ell = 1, \ldots, L \tag{6-2}$$

stating that all raw effluent from sector ℓ has to be accounted for. If the possibility of "no treatment" is allowed then it could also be included as a treatment process with zero cost.

$$\text{Minimize } Z = \sum_{\ell=1}^{L} \sum_{k=1}^{K_\ell} c_{k,\ell}\, x_{k,\ell} \tag{6-3}$$

stating that the total cost is to be minimized. It is also required that

$$x_{k,\ell} \geqq 0 \;\forall\; k , \ell . \tag{6-4}$$

The problem of minimizing the total cost Z subject to (6-1), (6-2), and (6-4) is a linear program for which rapid computer codes exist [33]. These codes not only provide the values of the decision variables $x_{k,\ell}$ but also give the simplex multipliers or shadow prices

$$\pi_m \ (m = 1, \ldots, M) \ , \ \mu_\ell \ (\ell = 1, \ldots, L) \ ,$$

which have very important economic interpretations.

π_m may be interpreted as the marginal increase in minimum cost per unit increase in b_m , the total allowable discharge of effluent component m ; μ_ℓ is the marginal increase in minimum cost per unit increase in d_ℓ , the total amount of untreated effluent from sector ℓ . Clearly from the nature of the problem, $\pi_m \leq 0 \; \forall \; m$ and $\mu_\ell \geq 0 \; \forall \; \ell$. If $\pi_m = 0$, this usually means that the amount of effluent m resulting from the optimum treatment program is strictly less than the allowable amount and still there is spare capacity in the basin to assimilate more of this effluent.

The economic advisability of any proposed new treatment may be determined using these dual or shadow prices. Suppose a new process $k = K_\ell + 1$ is being proposed for industry ℓ . Per unit of raw effluent processed, the new process leaves $a_{K_\ell+1,\ell,1}$ units of component 1, $a_{K_\ell+1,\ell,2}$ units of component 2, and so on at a new cost per unit of $c_{K_\ell+1,\ell}$. Using the marginal costs π_m and μ_ℓ , one can compute the net cost of processing one unit of raw effluent by this new process as

$$\Delta_{K_\ell+1} = c_{K_\ell+1,\ell} - \mu_\ell - \pi_1 a_{K_\ell+1,\ell,1} - \cdots - \pi_M a_{K_\ell+1,\ell,M} . \qquad (6\text{-}5)$$

If $\Delta_{K_\ell+1}$ is positive, this means that the combination of treatments previously being used are more efficient. But, if $\Delta_{K_\ell+1}$ is negative, this means that for small amounts of processing, the total cost is reduced by $\Delta_{K_\ell+1}$ for each unit of raw effluent processed by the $K_\ell + 1^{th}$ treatment. Other standard interpretations of solutions of linear programming problems are also applicable to this model.

The linear programming representation of the model is illustrated in Table VI. The application of this model has been demonstrated for the Suisun Bay-Lower San Joaquin River area in [34] and [5] using the data from the San Francisco Bay Comprehensive Study [35].

ECONOMIC GROWTH PROJECTIONS AND OTHER MODIFICATIONS

The model described in the preceding section may be extended to solve the problem of maintaining a desired water quality standard in a basin which is experiencing with time increasing discharges of effluent as a result of population and industrial growth. The necessary changes in the optimal policy as a function of time could be obtained by using a parametric programming approach [24].

Economic and demographic growth projections may be used to estimate the increase in the effluent flow vector d_ℓ from industrial and municipal dischargers. This projection of future effluent discharges would form new right-hand sides in the model, each representing a period. A simple approach, though only approximate, is to assume that the generation of raw effluent will be a linear function of industrial activity and population growth. Thus the raw effluent of each discharger is a piecewise linear function of time and could be solved as a linear program if the breakpoints are known.

By using the above approach, it should be possible to project future needs of waste treatment and consequently a plan of future investments may be drawn out. It may be expected that expensive treatment procedures would in time enter the optimum plan as the inexpensive methods would be inadequate in the face of growing demands. The need for investment in research to improve upon the existing production and treatment processes would also be pointed out by the increasing total cost of waste treatment to maintain a specified quality standard in the face of industrial and population growth.

The capacity of the estuarine basin for waste transportation depends on the volume flow in the estuary, and one way to counteract the growing pollution load is to increase volume flow by flow augmentation. If the water standard vector $b = (b_1, \ldots, b_m)$ is regarded as being determined relative to the mass flow Q , then flow augmentation f will increase b and this may be expressed as

$$b(f) = b + f\Delta\ell \qquad (6\text{-}6)$$

where $\Delta\ell$ is the vector of changes in b per unit flow. If $f\Delta\ell$ is subtracted from both sides of (6-1), a linear program is again obtained.

TABLE VI

LINEAR PROGRAMMING WATER QUALITY CONTROL MODEL IN TABLEAU FORM

Discharger	1	2		ℓ		
Variables $x_{k,\ell}$	x_{o1} x_{11} x_{21} ... x_{k1}	x_{o2} x_{12} x_{22} ... x_{k2}	...	$x_{o\ell}$ $x_{1\ell}$ $x_{2\ell}$ ... $x_{k,\ell}$		
Costs $c_{k,\ell}$	c_{o1} c_{11} c_{21} ... c_{k1}	c_{o2} c_{12} c_{22} ... c_{k2}	...	$c_{o\ell}$ $c_{1\ell}$ $c_{2\ell}$ ... $c_{k,\ell}$	Upper Bound	Shadow Prices
	a_{o11} a_{111} a_{211} ... a_{k11}	a_{o21} a_{121} a_{221} ... a_{k21}	...	$a_{o\ell 1}$ $a_{1\ell 1}$ $a_{2\ell 1}$ ... $a_{k,\ell 1}$	b_1	π_1
	a_{o12} a_{112} a_{212} ... a_{k12}	a_{o21} a_{122} a_{222} ... a_{k22}	...	$a_{o\ell 2}$ $a_{1\ell 2}$ $a_{2\ell 2}$ ... $a_{k,\ell 2}$	b_2	π_2
	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$
	a_{o1m} a_{11m} a_{21m} ... a_{k1m}	a_{o2m} a_{12m} a_{22m} ... a_{k2m}	...	$a_{o\ell,m}$ $a_{1\ell,m}$ $a_{2\ell,m}$ ... $a_{k,\ell,m}$	b_m	π_m
					Flow	
	1 1 1 ... 1				d_1	μ_1
		1 1 1 ... 1			d_2	μ_2
			$\ddots$		$\vdots$	$\vdots$
				1 1 1 ... 1	d_ℓ	μ_ℓ

If social costs are known as a function of the level of pollution of the various components, these could also be incorporated as in Model C, Chapter II. Let the social cost of pollution component m be a linear function $\partial_{om} + \partial_m Y_m$ of the total amount Y_m of component m present. But $Y_m = b_m - W_m = \sum_{\ell} \sum_{k} a_{k,\ell,m} x_{k,\ell}$, where W_m is the slack in the m^{th} inequality of (6-1). Hence the social cost due to component m is $\partial_{om} + \partial_m (b_m - W_m)$. As $\partial_{om} + \partial_m b_m$ is a constant, to include the social cost due to m it is only necessary to assign a cost coefficient of $-\partial_m$ to the slack variable W_m.

IMPLEMENTATION OF THE MODEL

There are various objections to a model which minimizes the total cost over the basin, not the least is that it is not equitable. The optimal solution usually picks up the industries and municipalities having highly efficient and low-cost treatment processes to do most of the treatment and removal of wastes. As a result, some industries may treat their effluent at a high level whereas other industries are allowed to discharge their effluent with little and sometimes no treatment at all. Still, it could be shown [5, 29] that the total treatment costs over the entire basin using the optimal solution is much lower than if all waste dischargers were treating their effluent at the same level, e.g., secondary treatment.

It is obvious that the implementation of the model herein proposed requires setting up a regional organization which would be responsible for allocating the total cost among the waste dischargers in some equitable fashion. One of the ways to effect this allocation of costs and to motivate the individual waste dischargers to implement the optimal solution is through a system of charges on effluents, discussed at great length by Kneese [1].

Suppose dischargers were taxed $-\pi_i$ times the amount of effluent component i remaining after treatment, $i = 1, 2, \ldots, M$. Then for the treatment process or processes which they should use in order to implement the optimal solution, the net cost per unit of effluent treated is

$$c_{k,\ell} - \sum_{m=1}^{M} \pi_m a_{k,\ell,m} = \mu_\ell \qquad (6\text{-}7)$$

and the net cost if any other treatment is used is

$$c_{k,\ell} - \sum_{m=1}^{M} \pi_m a_{k,\ell,m} \geqq \mu_\ell . \qquad (6\text{-}8)$$

Thus if the regional estuarine organization collects charges or taxes in this fashion, and the dischargers act to minimize their costs, they would tend to use the treatments suggested by the minimum cost solution for the entire basin.

From the duality theory of linear programming, the total taxes collected must equal the total cost of operation of all the treatment plants. The dischargers may either be disbursed for their job of waste treatment, or the organization may run the treatment plants itself. It may also decide to build and operate large-scale treatment plants common to more than one discharger. This system is equitable as the dischargers are paying a tax for discharging waste into the basin which is marginally equal to the cost of removing it. For the specific components with $\pi_i = 0$ there is spare capacity in the basin and no charge is being paid until the capacity is used up.

It is perhaps appropriate to summarize some of the departures from reality incurred due to the simplifying assumptions that have been made in the waste treatment model and indicate the degree of difficulty involved in more accurately modeling these aspects. Probably the most significant departure from reality is the requirement that the water quality standards be specified in terms of dischargers rather than concentration in the receiving water. As already explained, using this model in conjunction with a dispersion model, (e.g., Model B of Chapter V) would remove this difficulty. In the next chapter, an integration of the two models into a large linear program is presented. In some situations, the treatment cost functions may be nonlinear. A simple generalization is to allow piecewise linear and convex cost functions. These functions can be represented in linear terms [14]. Nonconvex cost functions or costs which involve fixed charges (i.e., capital charges for treatment facilities) lead to mixed integer programs which while easy to formulate [14] are difficult to solve. In some cases branch and bound methods [36] could be used to resolve these problems [37]. Uncertainties in the parameters of the problem can be attacked by the methods of stochastic programming [38].

VII. SYNTHESIS OF THE DISPERSION AND WASTE TREATMENT MODELS

INTRODUCTION

In Chapter V it is shown that, given the quality standards, the dispersion model generates a linear program for each quality constituent for obtaining optimal discharge plans along the estuary. In Chapter VI, a multicomponent waste treatment model is presented as a linear program which has to be solved for each section of the estuary. But if they are applied in succession as two distinct stages, there is a danger of suboptimization due to possible variations in treatment costs in different treatment plants. In the section which follows these two stages are integrated into a multicomponent water quality model which simultaneously provides optimal plans of treatment and discharge along the estuary. The resulting linear program is often large-sized and sophisticated techniques may be used to take advantage of the special structure of the coefficient matrix. Economics of alternative methods of quality improvement and cost reduction schemes like transportation of waste from one section of the estuary to another or process changes may also be studied in this model with addition of new activities. Economic growth projections and other modifications like inclusion of social costs, discussed in Chapter VI, may be incorporated in this model. The dual prices could be used as a basis for a system of charges aimed at equitable distribution of operating costs among dischargers and motivating them to reduce waste discharge by improvements in production and waste treatment processes. To keep the discussion simple, a steady state model for conservative substances will be illustrated, though it can be easily extended for decaying substances and unsteady state case.

MATHEMATICAL FORMULATION OF THE MODEL

Let the estuary be divided into n longitudinal reaches whose hydrological characteristics have been already determined and let there be M effluent components under consideration to characterize water quality.

Let c_i^m be the concentration of the m^{th} effluent at section i , $m = 1, 2, \ldots, M$; $i = 0, 1, \ldots, n$. If U_i^m is the maximum allowable value c_i^m can take, Equation (5-18) can then be rewritten as

$$c_{i+1}^m - d_i \, c_{i-1}^m + g_i \sum_{j=1}^{i} S_j^m + g_i \, F^m = 0 \qquad (7\text{-}1)$$

$$0 \leq c_i^m \leq U_i^m$$

$$i = 1, 2, \ldots, n-1$$

$$m = 1, 2, \ldots, M$$

the superscript m denoting quantities relating to the m^{th} component of water quality. Along with this are the corresponding equation and bounds for boundary sections.

$$\left.\begin{array}{l} 0 \leq c_o^m \leq U_o^m \\ \quad c_n^m - d_n \, c_{n-1}^m + g_n \sum_{i=1}^{n} S_i^m + g_n \, F^m = 0 \\ 0 \leq c_n^m \leq U_n^m \end{array}\right\} \quad m = 1, 2, \ldots, M . \qquad \begin{array}{r} (7\text{-}2) \\ \\ (7\text{-}3) \end{array}$$

The coefficients d_i , g_i , F , have the same interpretation as in Chapter V.

The notations of Chapter VI have to be modified to include a subscript denoting the reach of the estuary. Assume there are L_j industrial sectors in reach j of the estuary and that for each sector ℓ , there are $K_{j\ell}$ possible methods of effluent treatment.

$a_{j,k,\ell,m}$ = the amount of effluent component m released per unit of untreated effluent by the k^{th} treatment for sector (or industry) ℓ in the j^{th} reach.

$$k = 1, 2, \ldots, K_{j\ell} \; ; \; \ell = 1, 2, \ldots, L_j$$

$$m = 1, 2, \ldots, M \quad ; \; j = 1, 2, \ldots, n$$

$d_{j,\ell}$ = the total amount of untreated effluent (of known composition) produced by the industrial sector ℓ in reach j (in unit time).

$e_{j,k,\ell}$ = the cost of treating one unit of raw effluent (of known composition) from industry ℓ or reach j by treatment k .

The model will determine a set of decision variables $x_{j,k,\ell}$ interpreted by

$x_{j,k,\ell}$ = the amount of untreated effluent from industry ℓ of reach j treated by method k

in such a way that the total cost taken over all industrial sectors in all the reaches of the estuary is minimized. Now S_j^m , the amount of component m discharged in reach j in unit time is obtained by adding the effluent component m released by all treatment processes in an industry and summing again over all the industries or sectors discharging waste in reach j of the estuary,

$$S_j^m = \sum_{\ell=1}^{L_j} \sum_{k=1}^{K_{j\ell}} a_{j,k,\ell,m} \, x_{j,k,\ell} \; ; \quad m = 1, 2, \ldots, M \qquad (7\text{-}4)$$

$$j = 1, 2, \ldots, n \, .$$

Combining (7-4) with (7-1), (7-2), and (7-3) successively, the following equations for m = 1, 2, ..., M are obtained.

$$c_{i+1}^m - d_i \, c_{i-1}^m + g_i \sum_{j=1}^{i} \sum_{\ell=1}^{L_j} \sum_{k=1}^{K_{j\ell}} a_{j,k,\ell,m} \, x_{j,k,\ell} + g_i \, F^m = 0 \qquad (7\text{-}5)$$

$$0 \leq c_i^m \leq U_i^m$$

$$i = 1, 2, \ldots, n-1 \; ;$$

$$0 \leq c_o^m \leq U_o^m \qquad (7\text{-}6)$$

and

$$c_n^m - d_n \, c_{n-1}^m + g_n \sum_{j=1}^{n} \sum_{\ell=1}^{L_j} \sum_{k=1}^{K_{j\ell}} a_{j,k,\ell,m} \, x_{j,k,\ell} + g_n \, F^m = 0 \qquad (7\text{-}7)$$

$$0 \leq c_n^m \leq U_n^m \, .$$

To account for all raw effluent generated by industry ℓ in reach j , the following condition must be satisfied.

$$\sum_{k=1}^{K_{j\ell}} x_{j,k,\ell} = d_{j,\ell}\ ; \quad \ell = 1, 2, \ldots, L_j \qquad (7\text{-}8)$$

$$j = 1, 2, \ldots, n\ .$$

The total treatment cost Z given by the following equation has to be minimized.

$$Z = \sum_{j=1}^{n} \sum_{\ell=1}^{L_j} \sum_{k=1}^{K_{j\ell}} e_{j,k,\ell}\ x_{j,k,\ell}\ . \qquad (7\text{-}9)$$

It is also required from feasibility that

$$x_{j,k,\ell} \geq 0\ \forall\ j\ ,\ \ell\ ,\ k\ . \qquad (7\text{-}10)$$

(7-5) - (7-10) constitutes a linear program, (7-9) being the objective function to be minimized. New coefficients could be defined in (7-5) and (7-7) and these equations modified by substituting

$$b_{i,j,k,\ell,m} = g_i\ a_{j,k,\ell,m}\ ; \quad i = 1, 2, \ldots, n \qquad (7\text{-}11)$$

$$j = 1, 2, \ldots, n$$

$$\text{for } \forall\ k\ ,\ \ell\ ,\ m\ .$$

The linear programming representation of the model is illustrated in Table VII. Before discussing special methods of solution for this linear programming problem which has a regular structure, several additions and modifications of the model along with the interpretation of dual shadow prices are presented.

INTERPRETATION AND MODIFICATIONS OF THE MODEL

Dual Prices

The solution of the linear programming problem in the previous section, in addition to giving values of the variables c_i^m and $x_{j,k,\ell}$, also provides us with the values of the simplex multipliers or shadow prices

$$\pi_{im}\ (i = 1, 2, \ldots, n\ ; \quad m = 1, 2, \ldots, M)\ ,$$

$$\mu_{j\ell}\ (j = 1, 2, \ldots, n\ ; \quad \ell = 1, 2, \ldots, L_j)\ .$$

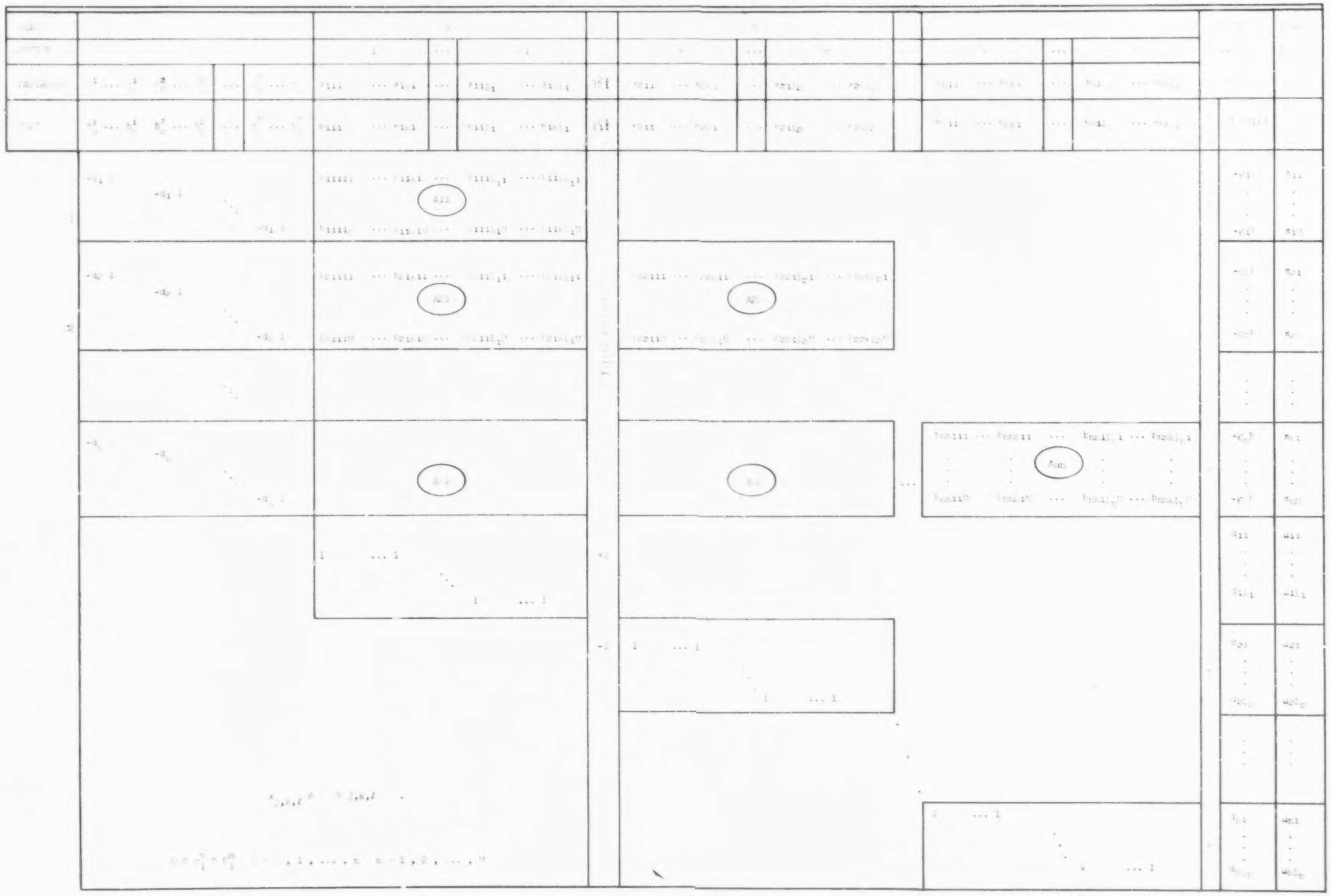
These shadow prices have similar interpretation to those given in Chapter VI, π_{im} now being the marginal cost of changing the given amount $g_i F^m$ and $\mu_{j\ell}$ that of changing the raw effluent quantity $d_{j\ell}$. The economic advisability of any proposed new treatment process could also be examined using these prices.

Economic Growth Projections

The same kind of parametric programming approach as discussed in Chapter VI may be used to obtain periodic optimal water quality control plans over time to account for increasing waste loads to be handled as a result of population and industrial growth in the future. Economic and demographic growth projections may be used to estimate the increases in effluent flow vectors $d_{j\ell}$ from industrial and municipal dischargers. If a stage-by-stage tightening of the water quality standards U_i^m is desired in the future in a highly polluted estuary, this could also be accomplished by a similar parametric programming approach or using multiple right-hand sides.

TABLE VII

LINEAR PROGRAMMING FORMULATION OF THE INTEGRATED DISPERSION AND TREATMENT MODEL


A11
A21
A22
Amn

Social Costs of Pollution

If social costs of pollution are known as a function of the level of concentration of the various components and the particular reach of the estuary, these could also be incorporated as in Chapter VI. The social cost of pollution due to the same component at the same level may vary from one reach of the estuary to another due to differences in water use and location.

Let the social cost of pollution due to component m at reach j (in between sections j-1 and j) be represented by a linear* function

$$\beta_j^m = \gamma_{oj}^m + \gamma_j^m \left[\alpha_j^m c_{j-1}^m + \left(1 - \alpha_j^m \right) c_j^m \right] \text{ for } j = 1, 2, \ldots, n \qquad (7\text{-}13)$$

where α_j^m may be usually given a value of 0.5 with $0 \leq \alpha_j^m \leq 1$. Hence the total social cost of pollution along the estuary is given by

$$TS_c = \sum_{j=1}^{n} \sum_{m=1}^{M} \beta_j^m = \sum_{j=1}^{n} \sum_{m=1}^{M} \gamma_{oj}^m + \sum_{m=1}^{M} \gamma_1^m \alpha_1^m c_o^m$$

$$+ \sum_{j=1}^{n-1} \sum_{m=1}^{M} \gamma_j^m c_j^m \left(1 - \alpha_j^m + \alpha_{j+1}^m \right) + \sum_{m=1}^{M} \gamma_n^m c_n^m \left(1 - \alpha_n^m \right) \qquad (7\text{-}14)$$

which is a linear function of the variables c_i^m representing constituent concentrations. The first term of (7-14) is constant and so it is only necessary to assign cost coefficients δ_i^m to the variables c_i^m with

$$\delta_o^m = \gamma_1^m \alpha_1^m$$

$$\delta_n^m = \gamma_n^m \left(1 - \alpha_n^m \right)$$

and

$$\delta_i^m = \gamma_i^m \left(1 - \alpha_i^m + \alpha_{i+1}^m \right), \; i = 1, 2, \ldots, n-1$$
$$m = 1, 2, \ldots, M \; . \qquad (7\text{-}15)$$

The coefficients δ_i^m have been used in Table VII as cost coefficients for social costs of pollution.

Transportation of Wastes by Piping

Throughout this chapter, it has been assumed that the raw effluent generated in an industry or municipality is treated by one or more treatment processes available to it and the resulting effluent is released at the nearest outfall in the nearest reach of the estuary. However, much benefit may be obtained by removing this restriction and allowing transportation of raw or treated effluent when economical.

Along certain parts of the estuary, there may be overcrowding of industries and/or highly populated cities resulting in very high waste-generation rates. To keep the adjacent reaches of the estuary at an acceptable level of quality most of the waste may have to be treated at higher levels at increasing cost. This may be averted by transporting raw or treated effluent to other sections of the estuary more favorable to waste disposal. Also economics of scale may be obtained by piping raw effluent from several cities or industries to a common large-scale treatment plant located at a suitable site along the estuary. Assuming the cost of transporting raw effluent from one sector of a reach to another sector of the same or a different reach is a linear function of the quantity transported, with the cost rate depending on the distance between them, such piping activities could be included in the general linear program. This is illustrated in Table VII as the piping activity at a cost rate p per unit flow. The column for this activity has entries (+1) in the $d_{j\ell}$-row for the sender and (-1) for the $d_{j\ell}$-row for the receiver. Any number of such activities for possible transportation routes may be included in the linear program though it might destroy the special structure of the matrix. Whether any particular route is economically feasible can be ascertained from the dual prices $\mu_{j\ell}$. It is clear that piping is only profitable if $(\mu_{j\ell})_{\text{sender}} - (\mu_{j\ell})_{\text{receiver}} \geq p$. Occasionally it may be possible to consider the possibility of transporting effluents directly to the ocean [40].

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*Damage costs due to fish kill show a linear relation to water quality in a study by Klein [39].

SOLUTION OF THE LINEAR PROGRAMMING MODEL

In Chapter V, it has already been noted that the multicomponent multisection model (Model C) of water quality control in an estuary developed into a large-scale linear program of formidable size. By integrating the two stages of the model into one linear program which incorporates the various treatment processes at all industries and municipalities, the size of the linear program has been further enlarged in this chapter. If expressed in the form $Ax = b$, the coefficient matrix A has $Mn + \sum_{j=1}^{n} L_j$ rows and $2\,Mn + \sum_{j=1}^{n} L_j K_{j\ell}$ columns where the symbols have been defined on page 69. If for a representative system it is assumed that $M = 10$, $n = 50$, $L_j = 10 \; \forall \; j$, and $K_{j\ell} = 7 \; \forall \; j , \ell$, there results a system with 1000 rows and 4000 columns. This is a very large system and special methods should be sought to solve this linear program rather than using a regular linear programming code.

The structure of the coefficient matrix is shown in Table VIII where the submatrices A_{ij} are similar to the upper half of the matrix presented in Table VI, and B_j are similar to the lower half. The submatrices C_i are similar to the left half of the matrix in Table IV. Again A_{ij}'s are arranged in the same fashion as the elements on the right half of the matrix in Table IV.

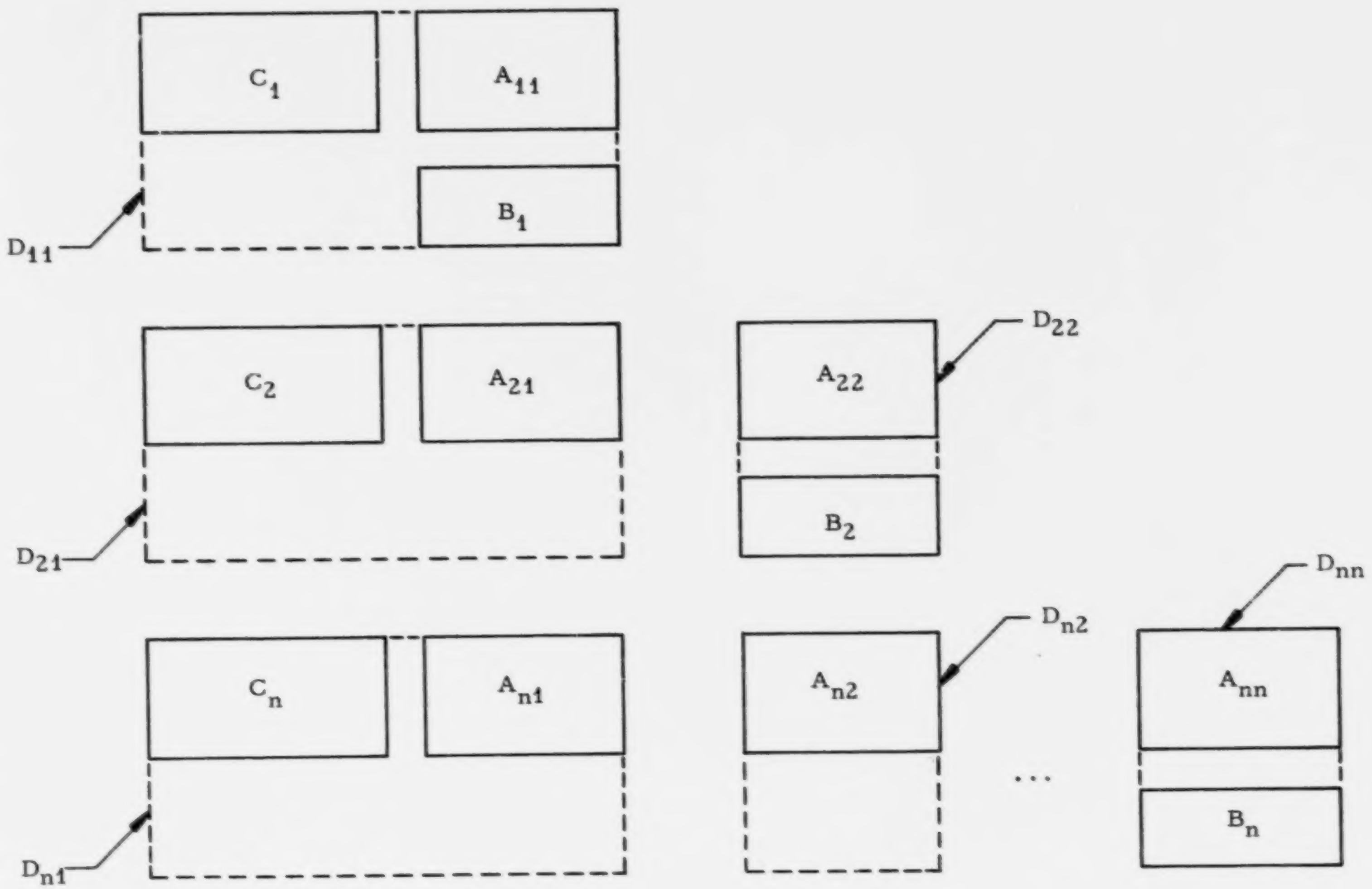
The regular structure of the coefficient matrix, as it appears in Table VIII, would suggest that it would be amenable to the Extension of Generalized Upper Bounded Techniques discussed by Sakarovitch and Saigal [41] and Kaul [42]. These techniques which are generalizations of the method of Dantzig and Van Slyke [33] define a working basis which is much smaller in size than the original basis and is used for most of the computation. However, a closer examination shows that these techniques will not have much advantage over the regular simplex method in this case. The efficiency of these techniques mostly depend on the assumption $L \gg m_o$ where L is the number of independent diagonal blocks and m_o is the number of linking equations. In our case, $L = n$ and $m_o = Mn$ and $m_o > L$. Hence the size of the working basis, given by m_o , is Mn as compared to $Mn + \sum_{j=1}^{n} L_j$, the size of the original basis. With the data assumed for a representative problem, the size of the working basis is only halved and it is still too large. Also these techniques will not take advantage of the block-triangular structure of the A_{ij}'s . Bennet's partitioning method [34] may be applied here. However, an alternative method for the solution of this problem is hereinafter proposed.

Method of Artificial Basis

The submatrices in Table VIII could be rearranged to obtain a block-triangular structure for the coefficient matrix. By "block-triangular" it is meant that if one partitions the matrix of coefficients into submatrices, these blocks, considered as elements, form a triangular system (see below). Let D_{tt} be a matrix with p_t columns and m_t rows

TABLE VIII

BLOCK TRIANGULAR ARRANGEMENT OF THE MATRIX OF TABLE VII


C_1
A_{11}
B_1
D_{11}
C_2
A_{21}
D_{21}
A_{22}
B_2
D_{22}
C_n
A_{n1}
D_{n1}
A_{n2}
D_{n2}
...
A_{nn}
B_n
D_{nn}

$$\begin{array}{llll} D_{00} & & & \\ D_{10} & D_{11} & & \\ D_{20} & D_{21} & D_{22} & \\ \cdot & & \cdot & \\ \cdot & & \quad\cdot & \\ \cdot & & \qquad\cdot & \\ D_{n0} & D_{n1} & D_{n2} & D_{nn} \end{array}$$

$(t = 0, 1, \ldots, n)$. Column vectors P_j , which have elements in common with D_{tt} , along with the corresponding variables, will be considered as belonging to the t^{th} period. Similarly for the equations.

The basis for this system has a block-triangular structure and hopefully differs from a square-block-triangular system in only a few columns. From the experience in solving dynamic Leontief models with substitution [43], it is known that a square-block-triangular basis has immense computational advantages. A solution method would be developed using an "artificial" square-block-triangular basis, motivated by Dantzig's work on block-triangularity [44].

The simplex method [14] will be applied through the use of an "artificial basis" $\overline{B}$ and a "true basis" B . The artificial basis will be square-block-triangular, and its inverse can be stored compactly by storing only the inverses of the submatrices forming the basis. As many columns of $\overline{B}$ as possible will be made the same as B .

Any column P_α of $\overline{B}$ can be expressed as a linear combination of the columns P_{ji} of B as

$$P_\alpha = \sum_{i=o}^{m} \eta_{i\alpha} P_{ji} , \; P_{jo} \equiv P_o \qquad (7\text{-}16)$$

and

$$B = \overline{B}\, \eta^{-1} \qquad (7\text{-}17)$$

is obtained where η is a (transformation) matrix whose α^{th} column has coefficients $\eta_{i\alpha}$. For columns common to both B and $\overline{B}$, η will have unit vectors. The few essential columns of η will consist of the columns which give the representation in terms of P_{ji} of those vectors $P_{\alpha i}$ in $\overline{B}$ and not in B . These vectors will be called artificial. η is stored along with the inverses of submatrices of $\overline{B}$ in a compact form, by storing only the essential columns, and their positions.

In the standard application of the revised simplex method [14], it is customary to maintain the inverse of the current basis (or the inverse in product form) in order to determine the set of simplex multipliers or pricing vectors π and the representation Y of the vector P_s entering the next basis in terms of the vectors of the current basis. The following relations are used for this purpose

$$\pi B = [1, 0, \ldots, 0] \;\; \text{(during Phase II)} \qquad (7\text{-}18)$$

and

$$Y = B^{-1} P_s \, . \qquad (7\text{-}19)$$

These relations, when changed for the artificial basis $\overline{B}$, take the form

$$\pi \overline{B} = [1, 0, \ldots, 0]\, \eta \qquad (7\text{-}20)$$

and

$$\overline{Y} = \overline{B}^{-1} P_s \; ; \quad Y = \eta\, \overline{Y} = \eta\, \overline{B}^{-1} P_s \qquad (7\text{-}21)$$

where $\overline{Y}$ is the representation of the vector entering the next basis in terms of the current artificial basis $\overline{B}$.

For doing operations with $\overline{B}$ as matrix, it is only necessary to store the inverses of the smaller diagonal submatrices of $\overline{B}$, denoted by $\overline{B}_{00}$, $\overline{B}_{11}$, etc. For example, in solving (7-21), the inverse of $\overline{B}_{00}$, when multiplied by the first m_0 components of the right-hand row vector P_s, will give the first m_0 components of $\overline{Y}$. Because of triangularity, these values can be substituted into equations associated with the next period and the next m_1 components of $\overline{Y}$ obtained through application of the inverse of $\overline{B}_{11}$, etc. The advantages of this compared with maintaining the entire basis $\overline{B}^{-1}$ (or B^{-1}) are considerable.

At each iteration, the true basis will change as a vector $P_{jr} \in B$ will be replaced by a vector P_s. The representation of P_{jr} in terms of the vectors of the new basis is given by

$$P_{jr} = \sum_{i \neq r} - \frac{y_i}{y_r} P_{ji} + \frac{1}{y_r} P_s \qquad (7\text{-}22)$$

where y_i are the components of Y. By substituting the expression (7-22) for P_{jr} in (7-16), the vector P_α can be reexpressed in terms of the next basis. Hence, if the "artificial" basis $\overline{B}$ is kept the same, these relations show the tranformation of η from one iteration to the next. One of the following three cases will arise depending on the positions of the columns P_{jr} and P_s.

Case 1: If P_{jr}, the vector replaced was also in $\overline{B}$, i.e., a vector common to both B and $\overline{B}$, then in the next cycle, P_{jr} will be an "artificial" vector if the same $\overline{B}$ is maintained and η will have one extra essential column and (7-22) will be maintained.

Case 2: If P_{jr} was not in $\overline{B}$ then (7-22) is of no interest and may be discarded. Here η retains the same size, if the same $\overline{B}$ is maintained.

Case 3: If P_s was artificial in $\overline{B}$, then the size of η would decrease by one, i.e., there will be one less "essential" column.

It is desirable to keep the number of essential columns of η as low and the structure of η as compact as possible, because the efficiency of the method will be taken away if η becomes too large. Hence, the possibility of changing $\overline{B}$, whenever the size of η can be reduced by this change, should be considered.

Let P_β be a column of B, not in $\overline{B}$, belonging to period t and suppose there are other artificial vectors also belonging to this period. The partitioned part of P_β belonging to period t can be represented in terms of the columns of $\overline{B}_{tt}$ by

$$P_\beta^{(t)} = \overline{B}_{tt} \, \overline{Y}^{(t)} . \qquad (7\text{-}23)$$

Now, if any of the components of $\overline{Y}^{(t)}$, corresponding to artificial column vectors P_α, is nonzero, then P_β can replace the corresponding P_α in $\overline{B}$ and still maintain the new $\overline{B}$ nonsingular. In this process, the size of the essential part of η is reduced and $\overline{Y}^{(t)}$ can also be used to obtain the updated inverse of $\overline{B}_{tt}^{-1}$, as in the regular simplex routine.

Because of the block triangularity of the original matrix, the representation of P_s (belonging to period t) in terms of $\overline{B}$ by (7-21) has already yielded the representation of $P_s^{(t)}$ in terms of the columns of $\overline{B}_{tt}$, i.e., the relation (7-23) required to determine if P_s can replace an artificial vector in $\overline{B}$. Therefore, it is not necessary to make a separate calculation to determine this. These relations (7-23) may be saved and updated when the columns of B_{tt} change, so that these are readily available. Thus if η could be kept compact, this method might be quite efficient compared with the regular simplex method for solving the large-scale system representing the Integrated Water Quality Model.

DISCUSSION

The main advantages of the integrated dispersion and waste treatment model are its multicomponent nature, availability of standard computer codes for fast solution, direct output of optimum treatment plans, and concentration profiles, flexibility in using for various diverse objectives such as studying future quality control and investment needs or the economic desirability of piping effluent within the reach of the estuary or away from it.

Inasmuch as industrial, domestic, and agricultural discharges contain many toxic and/or stable chemical compounds (some of which may have as yet unknown harmful effects on human health and marine ecology), the need for multicomponent water quality standards cannot be overemphasized. As any treatment process simultaneously acts on most of the constituents present in the effluent and effluents vary in their composition for each waste discharger, a model that can simultaneously handle all the quality constituents is essential if optimal combination of treatment processes is desired. Most of the past work lacked this aspect of the problem before Carew and Van Slyke [29] developed a multicomponent linear programming model. As discussed in Chapter VI, some of the limitations of their model have been removed in this chapter by integrating it with a dispersion model.

Critical appraisal of the Dispersion Models in relation to other existing models of water quality control has been presented in Chapter V and the same comments are also applicable for the model developed in this chapter.

Appendix C presents an illustration of the integrated dispersion and waste treatment model in the Suisun Bay-Lower San Joaquin River area where phosphate and BOD are treated as water quality factors.

VIII. SUMMARY AND CONCLUSIONS

SUMMARY

In this report, a multicomponent model of water quality control in an estuary is developed. Given a prescribed water quality standard in an estuary, expressed as maximum allowable concentrations of multiple water quality constituents, this model obtains an optimal plan of effluent treatment by waste-producing agencies, along with an optimal plan of effluent discharge in the estuary by minimizing the total cost of pollution abatement for the estuarine region.

The physical system of waste transport and degradation in an estuary is described by a one-dimensional diffusion equation. Dispersion models A, B, and C are developed for optimal allocation of water quality in an estuary to obtain different but related objectives. These models are characterized as linear optimal control problems under steady state assumptions in the estuary. A duality relation between models A and B is explored to show that a solution of one is also a solution of the other model.

Certain basic results of linear optimal control theory and the related minimum principle are developed. These are then applied to obtain general solutions for optimization models B and C. The behavior of the optimal discharge policy in relation to the functions representing hydrological variables such as volume flow and cross-sectional area of the estuary is discussed.

The discrete versions of models A, B, and C are developed with a view to using the discrete data available from sampling studies in the estuary. They generate linear programs under both steady state and nonsteady state assumptions.

A waste treatment model is presented which generates an optimal waste treatment plan for all waste-producing agencies in the region by minimizing the total waste treatment costs.

Finally, the complete model of estuarine water quality management developed in the report is obtained by a synthesis of Dispersion Model B and the waste treatment model. A modification of the simplex method is discussed which takes advantage of the regular structure of the large-scale linear program generated to reduce computational effort. Economic interpretations and modifications are discussed. Illustrations of this model and of Model B in the Suisun Bay of the San Francisco Bay system is also presented.

CONCLUSIONS

While developing a model of estuarine water quality control, one has to work within the limited boundaries of knowledge about water pollution, waste treatment, and mixing processes in estuaries and much is desired in terms of understanding these processes so that they can be described in precise mathematical terms.

Development of a two-dimensional estuarine dispersion model is reported in [31] but still the estimation of the dispersion coefficients presents formidable problems. Harleman [7] proposes a theoretical expression for estimating a longitudinal dispersion coefficient from hydrological parameters in the estuary, but still no reliable theoretical method is available for most estuarine situations. Additional research is needed to develop a three-dimensional description of the dispersion process along with a method of estimating directional dispersion coefficients.

Movement and resulting concentration of conservative substances can be described adequately if a proper description of the dispersive and advective processes is available. However, for nonconservative constituents the accuracy of a model is dependent to a great extent on the reliability of the estimates of the reaction rate constants. Usually these estimates are arrived at by subjective judgments based on the experience of the investigator with the particular environment and waste discharges. There is a need to seek better mathematical descriptions of nonconservative processes, particularly of the biological reactions.

A need for continual search for more efficient, complete, and inexpensive treatment processes cannot be overemphasized. The optimal operation and control of treatment processes is by itself a challenging field.

The solutions of the water quality control model proposed herein is sensitive to the water quality standards used. Multicomponent water quality standards are still not available for many estuarine basins. The harmful effects of many constituents by themselves or in conjunction with other constituents on human health and marine ecology are not yet completely understood in quantitative terms. Further research and legislation are needed for establishing proper water quality standards.

Quantitative information regarding harmful effects and social costs of pollution and benefits from quality improvement projects are lacking today so that these costs and benefits cannot be included in optimization models. In the report the author has developed deterministic models and considered concentrations averaged over one or more complete tidal cycles. In unsteady state models, only long-term or seasonal variations are considered. Stochastic models may be developed to study variations of water quality during a tidal cycle and effects of random variations of volume of flow in the estuary. There has been some progress in this direction.

Finally there is a need to consider environmental pollution as an integral problem, whether it is in the water, in the air, or in the form of solid wastes. Public awareness and public education about the desirability of a congenial environment may be a necessary step toward creating a better world for all of us.

APPENDICES

APPENDIX A

A DISCRETE STEADY STATE FORMULATION OF THE DISPERSION MODEL FOR DEGRADABLE CONSTITUENTS

In Chapter V the discrete steady state formulation of dispersion models for conservative constituents has been described. In this section, necessary modifications will be made for decaying constituents (like BOD) where the decaying process could be described by a first-order reaction.

The steady state dispersion equation for a degradable constituent may be written from (2-9) and the boundary conditions as

$$\frac{dc(x)}{dx} = \frac{v}{E} c(x) - \frac{1}{AE}\left\{\int_0^x S\,dx - \int_0^x (kAc)dx + F\right\} \qquad \text{(A1)}$$

where k = first order decay rate constant and F = transport rate across the boundary at origin for the decaying constituent.

Using the forward finite difference scheme and substituting $\left(\frac{dc}{dx}\right)_i = \frac{c_{i+1} - c_i}{x_{i+1}}$, one obtains

$$\frac{c_{i+1} - c_i}{x_{i+1}} = \frac{v_i}{E_i} c_i - \frac{1}{A_i E_i}\left\{\sum_{p=1}^{i} S_p + F - k\sum_{j=1}^{i} A_j x_j c_j\right\}, \qquad i=0,\ 1,\ 2,\ \ldots,\ n-1 \qquad \text{(A2)}$$

which reduces to

$$c_i d_i - c_{i+1} - g_i\left(\sum_{p=1}^{i} S_p + F\right) + k g_i \sum_{j=1}^{i} A_j x_j c_j = 0 \qquad \text{(A3)}$$

where $d_i = \frac{E_i + x_{i+1} v_i}{E_i}$ and $g_i = \frac{x_{i+1}}{A_i E_i}$, $i=0,\ 1,\ 2,\ \ldots,\ n-1$.

From (A3), equations relating c_i to c_{i+1} and cumulative discharge rate at section i can be obtained.

As (A3) cannot be used for the n^{th} section and hence does not involve S_n, an additional equation is obtained for the n^{th} section using the backward difference scheme

$$\left(\frac{dc}{dx}\right)_n = \frac{c_n - c_{n-1}}{x_n} = \frac{v_n}{E_n} c_n - \frac{1}{A_n E_n}\left\{\sum_{p=1}^{n} S_p + F - k\sum_{j=1}^{n} A_j x_j c_j\right\} \qquad \text{(A4)}$$

which reduces to

$$c_n d_n + c_{n-1}\bar{d}_{n-1} - g_n\left(\sum_{p=1}^{n} S_p + F\right) + k g_n \sum_{j=1}^{n-2} A_j x_j c_j \qquad \text{(A5)}$$

where

$$d_n = \frac{x_n v_n}{E_n} + k\frac{x_n}{E_n} - 1$$

$$\bar{d}_{n-1} = 1 + \frac{k\ x_n A_{n-1}}{A_n E_n}$$

$$\bar{e}_n = \frac{x_n}{A_n E_n} .$$

Equations (A3) and (A5) describe the steady state dispersion process for decaying substances and now they can be substituted in Problems A, B, and C, along with appropriate bounds on c_i, to obtain linear programs. In case the decay constant k varies from section to section, (A3) and (A5) could be easily modified to accomodate this.

APPENDIX B

A DISCRETE NONSTEADY STATE FORMULATION OF THE DISPERSION MODEL FOR A CONSERVATIVE CONSTITUENT

The discrete nonsteady state formulation of the dispersion model has been discribed in Chapter V. Here the actual form of Equation (5-31), which describes the linear process, is defined. From (5-29)

$$c_{i,j+1} = c_{i,j} + \frac{t_{j+1} - t_j}{A_{i,j}} \left[\left(\frac{\partial}{\partial x}\left(AE \frac{\partial c}{\partial x} \right) \right)_{i,j} - \left(\frac{\partial}{\partial x} (Avc) \right)_{i,j} + (S)_{i,j} \right]$$

where $(S)_{i,j}$ is given by (5-30).

Employing the forward difference scheme and referring to Figure 9, the individual terms of (5-29) may be approximated as shown below:

I. $$\left[\frac{\partial}{\partial x}\left(AE \frac{\partial c}{\partial x} \right) \right]_{i,j} = \frac{1}{x_i - x_{i-1}} \left[\left(AE \frac{\partial c}{\partial x} \right)_{i+\frac{1}{2},j} - \left(AE \frac{\partial c}{\partial x} \right)_{i-\frac{1}{2},j} \right]$$

$$= \frac{1}{x_i - x_{i-1}} \left[(AE)_{i+\frac{1}{2},j} \left(\frac{\partial c}{\partial x} \right)_{i+\frac{1}{2},j} - \tfrac{1}{2}(A_i E_{i,j} + A_{i-1}E_{i-1,j}) \frac{(c_{i,j} - c_{i-1,j})}{(x_i - x_{i-1})} \right] .$$

Define $a_i = \dfrac{1}{x_i - x_{i-1}}$; $b_i = \dfrac{x_i - x_{i-1}}{x_{i+1} - x_i}$. Thus

$$(AE)_{i+\frac{1}{2},j} = A_i E_{i,j} + \frac{b_i}{2} (A_{i+1}E_{i+1,j} - A_i E_{i,j}) \quad \text{, and}$$

$$\left(\frac{\partial c}{\partial x} \right)_{i+\frac{1}{2},j} = a_i(c_{i,j} - c_{i-1,j}) + 2b_i\{a_{i+1}(c_{i+1,j} - c_{i,j}) - a_i(c_{i,j} - c_{i-1,j})\} \quad .$$

Define $e_{i,j} = A_i E_{i,j} + A_{i-1}E_{i-1,j}$; $d_{i,j} = A_i E_{i,j} + \frac{b_i}{2} e_{i+1,j}$.

On substitution,

$$I = a_i[d_{i,j}\{a_i(c_{i,j} - c_{i-1,j}) + 2b_i[a_{i+1}(c_{i+1,j} - c_{i,j}) - a_i(c_{i,j} - c_{i-1,j})]\}$$

$$- \frac{a_i}{2} e_{i,j}(c_{i,j} - c_{i-1,j})] = 2b_i a_i a_{i+1} d_{i,j} c_{i+1,j} + a_i\Big\{d_{i,j}(a_i - 2b_i a_{i+1} - 2b_i a_i)$$

$$- \frac{a_i}{2} e_{i,j}\Big\} c_{i,j} + a_i^2 \Big\{d_{i,j}(2b_i - 1) + \frac{e_{i,j}}{2}\Big\} c_{i-1,j} \quad .$$

II. $$\left(\frac{\partial}{\partial x} (Avc) \right)_{i,j} = \frac{1}{2(x_i - x_{i-1})} \left[(Avc)_{i+1,j} - (Avc)_{i-1,j} \right]$$

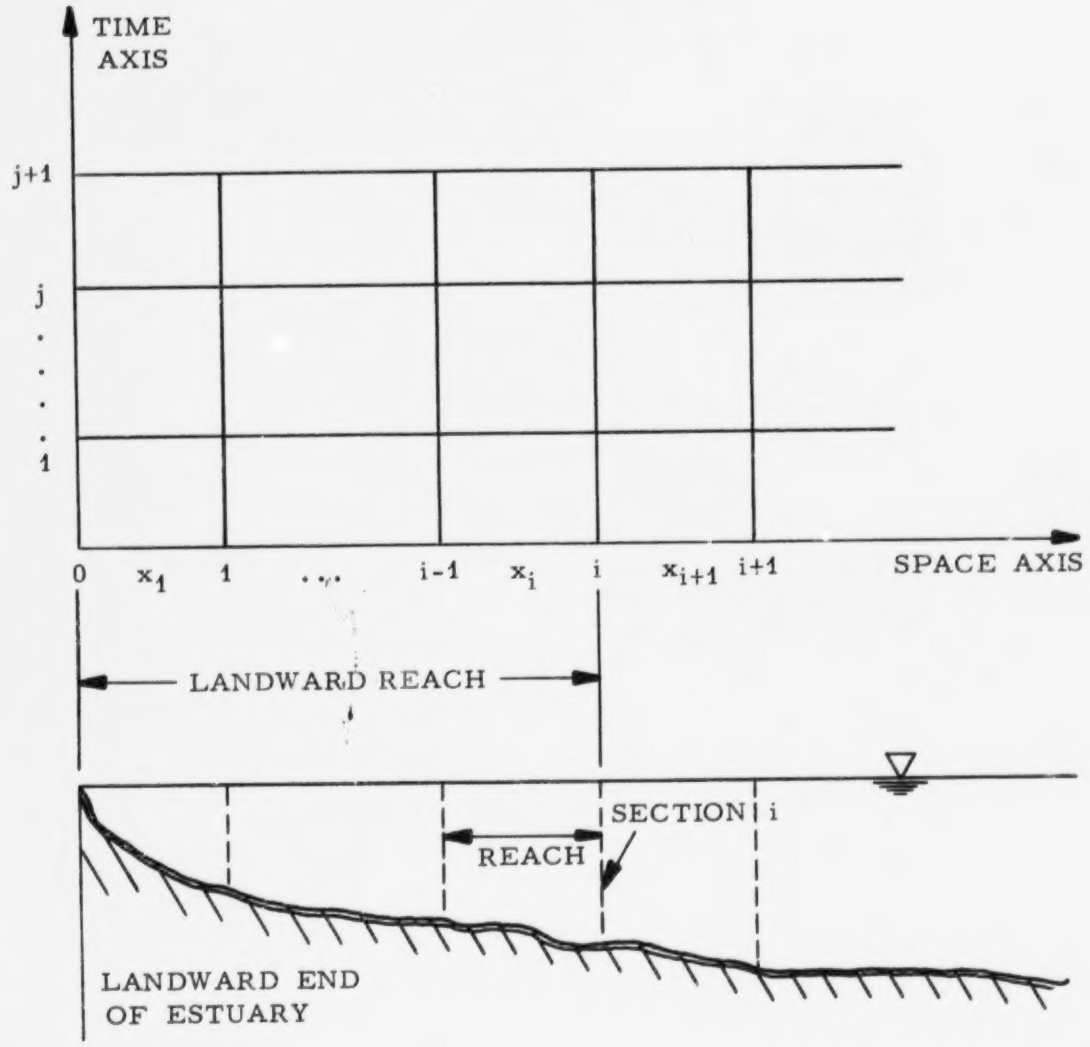

TIME
AXIS
j+1
j
1
0
x_1
1
...
i-1
x_i
i
x_{i+1}
i+1
SPACE AXIS
LANDWARD REACH
SECTION i
REACH
LANDWARD END
OF ESTUARY

FIGURE 9. FINITE DIFFERENCE SCHEME

where $(Avc)_{i-1,j} = A_{i-1}v_{i-1,j}c_{i-1,j}$ and

$$(Avc)_{i+1,j} = A_i v_{i,j}c_{i,j} + b_i(A_{i+1}v_{i+1,j}c_{i+1,j} - A_i v_{i,j}c_{i,j}) \ .$$

Defining $r_i = \frac{a_i}{2}(1 - b_i)$ we obtain on substitution

$$\text{II} = \frac{a_i}{2} A_{i+1}v_{i+1,j}c_{i+1,j} + r_i A_i v_{i,j}c_{i,j} - \frac{a_i}{2} A_{i-1}v_{i-1,j}c_{i-1,j} \ .$$

III. $(S)_{i,j} - (S_s)_{i,j} - (Q_L)_{i,j}\, c_{i,j} - k_{i,j}A_{i,j}c_{i,j}$ from (5-30).

Define $\Delta_{i,j} = \frac{t_{j+1} - t_j}{A_{i,j}}$. Hence, we obtain from (5-29) by substitution

$$\begin{aligned} c_{i,j+1} &= c_{i,j} + \Delta_{i,j}[\text{I} - \text{II} + \text{III}] \\ &= c_{i-1,j}\left[a_i^2\left\{d_{i,j}(2b_i - 1) + \frac{e_{i,j}}{2}\right\} + \frac{a_i}{2} A_{i-1}v_{i-1,j}\right]\Delta_{i,j} \\ &\quad + c_{i,j}\left[1 + \Delta_{i,j}a_i\left\{d_{i,j}(a_i - 2b_i a_{i+1} - 2b_i a_i) - \frac{a_i}{2} e_{i,j}\right\}\right. \\ &\quad \left. - \Delta_{i,j}\{r_i A_i v_{i,j}c_{i,j} + (Q_L)_{i,j} + k_{i,j}A_{i,j}\}\right] \\ &\quad + c_{i+1,j}\left[2b_i a_i a_{i+1}d_{i,j} - \frac{a_i}{2} A_{i+1}v_{i+1,j}\right]\Delta_{i,j} - \Delta_{i,j}(S_s)_{i,j} \ . \end{aligned}$$

On simplification, we have

$$c_{i,j+1} = f_{i,j}c_{i-1,j} + g_{i,j}c_{i,j} + h_{i,j}c_{i+1,j} - \Delta_{i,j}(S_s)_{i,j} \tag{5-31a}$$

where the constants $f_{i,j}$, $g_{i,j}$, and $h_{i,j}$ are appropriately defined above.

From the nature of Equation (5-31a), it may be noted that the linear program generated by using this equation will have a block-diagonal structure, one block for each time period and each block having a staircase structure. This would help in using better techniques for solving this linear program, which may become very large-sized.

APPENDIX C

ILLUSTRATION OF DISPERSION MODEL B AND INTEGRATED DISPERSION AND TREATMENT MODEL

In order to illustrate the models presented in this report, their application in an estuary is herein presented along with details of the necessary calculations and summary of results and comments.

The estuarine region chosen for this illustration is Suisun Bay in the northern branch of the San Francisco Bay system. The landward end is not easily defined, but for the purposes of this study is taken at the confluence of the San Joaquin and Sacramento rivers at the eastern end of Suisun Bay. A section west of the Benicia-Martinez Bridge is taken here as the seaward end, though for implementation purposes this boundary should be beyond the Golden Gate Bridge, and San Pablo Bay and Central San Francisco Bay should be included in the region of study.

The estuarine region in Suisun Bay is divided into 11 estuarine reaches by 12 sections through the deep-water sampling stations and points midway between them. These sections are listed in Table IX along with pertinent hydrological data needed for the models. Hydrological data collected and estimated during "A Comprehensive Study of San Francisco Bay" [12] is being used here.

The application of the Dispersion Model B in Suisun Bay is demonstrated for a conservative constituent – total phosphate. The maximum amount of phosphate that could be discharged in this region is obtained for differing quality standards and different assumptions regarding the minimum and maximum discharge rates at each segment of the estuary.

Carew and McGauhey [5] illustrate their "Linear Programming Water Quality Control Model" in the same estuarine region (Suisun Bay). The same waste generation and treatment cost data are being used here for illustrating the Integrated Dispersion and Waste Treatment Model developed in Chapter VII.

DISPERSION MODEL B

The steady state Dispersion Model B for a conservative constituent has been formulated as a linear program in Chapter V. Solution of Model B provides an optimal discharge plan which will maximize the total amount D of the constituent discharged in the estuarine region without violating a given quality standard (expressed as maximum allowable concentration for the constituent). Phosphate was chosen as the constituent for the study and it was assumed that transport of phosphate across the landward boundary is negligibly small (i.e., $F = 0$).

The linear program is described by Equations (5-12) through (5-15) in Chapter V. The cross-sectional area, A_i ; dispersion coefficient, E_i ; advective velocity, v_i ; and length of the segment, x_i , are tabulated in Table IX for sections 0 through 11. The coefficients f_i , g_i and d_i are computed using the appropriate relations (Equation (5-3)). The concentration of phosphate at section i is given by c_i and expressed in miligrams per liter (mg/ℓ), whereas the discharge rate at reach i, given by S_i , is expressed in pounds per day (lb/day). Thus g_i , as computed in Table IX in sec/ft^3, should be multiplied by a unit conversion factor 0.184337 to give $\bar{g}_i$; d_i and $\bar{g}_i$ should be used as the coefficients in the linear program. The structure of the linear programming tableau is shown in Table IV (Chapter V). The coefficient matrix has 11 rows and 23 columns not counting the bounds on the variables, as all c_i will have upper bounds and S_i may have both lower and upper bounds.

TABLE IX

HYDROLOGICAL DATA AND COEFFICIENTS FOR DISPERSION MODEL B IN SUISUN BAY

Section No. i	A_i $10^6 ft^2$	E_i ft^2/sec	v_i $10^{-3} ft/sec$	x_i $10^3 ft$	$Q_i = A_i v_i$ $10^3 ft^3/sec$	f_i 10^3	g_i 10^{-3}	d_i	$\bar{g}_i$ 10^{-4}
0	0.122	1000	12.3	-	1.5006	-	-	-	-
1	0.128	(850)[a]	11.7	9.85	1.4976	6.646	0.1712	1.1376	0.3155
2	0.104	700	(17.7)[a]	8.60	1.845	5.174	0.3019	1.5621	0.5515
3	0.135	(550)	10.9	8.60	1.4715	5.303	0.2618	1.3882	0.4826
4	0.217	400	(6.55)	7.80	1.4215	6.275	0.2060	1.2929	0.3798
5	0.216	(325)	6.35	7.80	1.3716	5.413	0.2474	1.3392	0.4560
6	0.383	250	(3.31)	7.05	1.2665	7.042	0.1624	1.1435	0.2994
7	0.202	(375)	5.75	7.05	1.1615	7.000	0.1712	1.1985	0.3156
8	0.216	500	(5.27)	4.75	1.1394	11.937	0.0926	1.1054	0.1707
9	0.194	(650)	5.76	4.75	1.1174	11.245	0.0987	1.1103	0.1820
10	0.162	800	(6.89)	7.05	1.1170	9.750	0.1158	1.1293	0.2135
11	0.175	(1050)	6.38	7.05	1.1165	-	0.0401	1.0448	0.0739

[a] Figures in paranthesis have been extrapolated from other data.

$$\left.\begin{aligned} f_i &= A_i \left\{ \frac{E_i}{x_i + x_{i+1}} + \frac{v_i}{2} \right\} \\ g_i &= \frac{2(x_i + x_{i+1})}{A_i [2E_i - v_i (x_i + x_{i+1})]} \\ d_i &= g_i f_i \\ \bar{g}_i &= 0.184337\, g_i \end{aligned}\right\} \quad i = 1, 2, \ldots, 10$$

$$g_{11} = \frac{x_{11}}{A_{11} (E_{11} - x_{11} v_{11})} \qquad d_{11} = \frac{E_{11}}{E_{11} - x_{11} v_{11}}$$

Once the basic linear program is ready, various questions may be asked, usually by changing the bounds on the variables.

1. The concentration of total phosphate in Suisun Bay—Lower San Joaquin River was found to range from 0.1 to 0.5 mg/ℓ during "A Comprehensive Study of San Francisco Bay" [35, Table 4-3]. Initially a value of 0.4 mg/ℓ was chosen as U_c , the maximum allowable concentration for all sections. From the physical nature of Dispersion Model B, it is expected that if there are no upper bounds on the amount discharged in a segment, the optimal solution would be to discharge as much as possible at the last segment near the ocean. This was confirmed by the model and it was found that a maximum amount of 59789.5 lb/day of phosphate could be discharged this way. The same upper bound $\overline{S}$ was then applied on all S_i and the magnitude of $\overline{S}$ was then varied (keeping U_c constant) and the maximal value of the total discharge D was found to be increasing with $\overline{S}$, though at a rate lower than the rate of increase of $\overline{S}$, as shown in the first five rows of Table X. A typical optimal discharge plan and the corresponding concentration profile for U_c = 0.4 mg/ℓ and $\overline{S}$ = 1500 lb/day is presented in Figure 10.

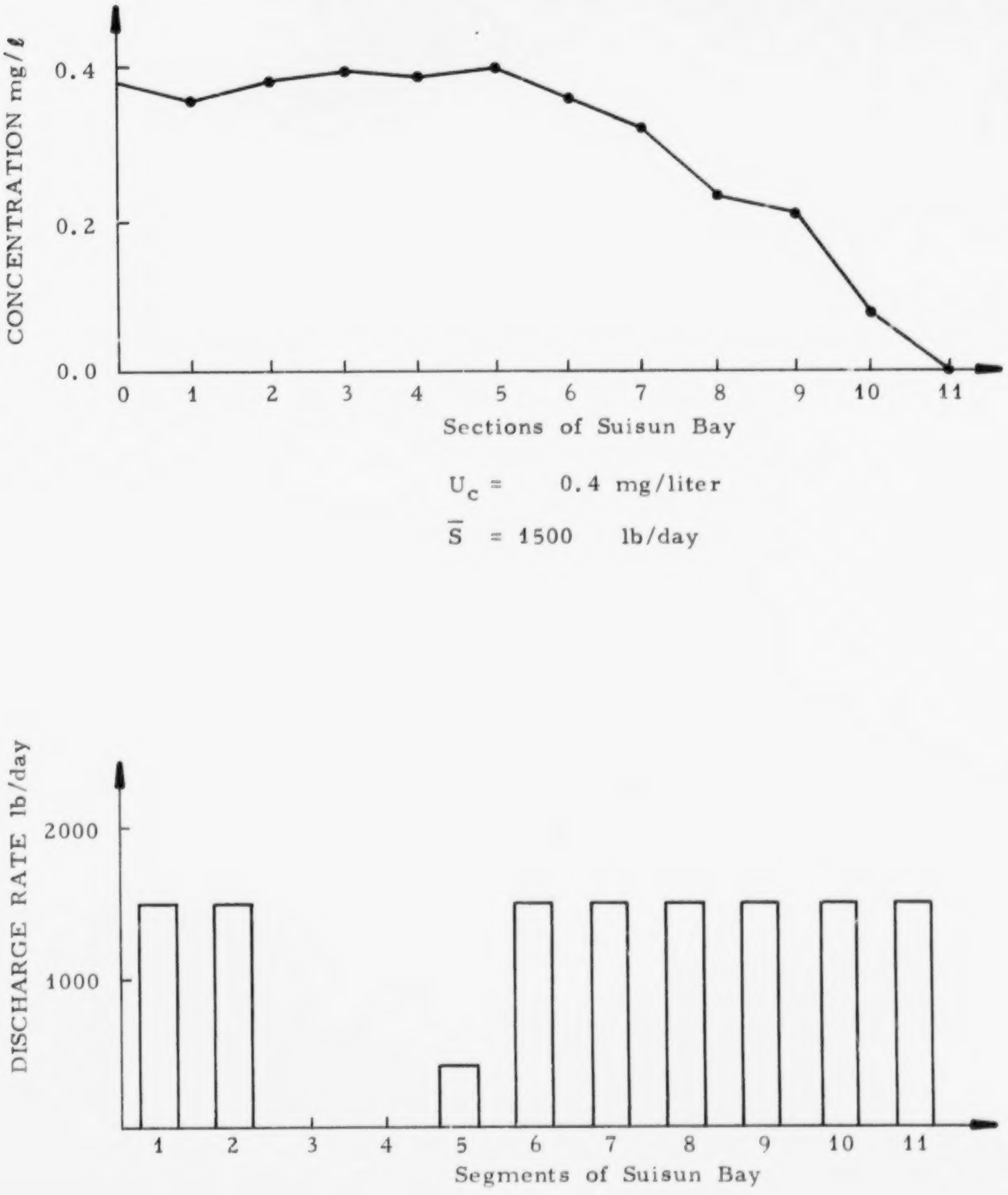
2. It is expected that D will be an increasing function of U_c , the upper bound on concentration of the constituent. U_c was varied from 0.2 mg/ℓ to 0.6 mg/ℓ (keeping $\overline{S}$ constant at 5000 lb/day) and the corresponding variation of D is expressed in the last three rows of Table X. It is to be noted that D is increasing at a rate lower than the rate of increase of U_c .

TABLE X

VARIATION OF D WITH $\overline{S}$ AND U_c

Serial Number	U_c mg/ℓ	$\overline{S}$ lb/day	D lb/day
1	0.4	1,500	12436.6
2	0.4	3,000	17552.7
3	0.4	5,000	22034.8
4	0.4	10,000	31156.0
5	0.4	∞	59789.5
6	0.2	5,000	15578.0
7	0.4	5,000	22034.8
8	0.6	5,000	28034.4

3. As each segment of the estuary may have waste generation activities within its reach, it may be necessary to discharge at least a part of it, if complete treatment or transportation to other reaches of the estuary is not possible. Lower bounds $\underline{S}_i$ on S_i are used for this purpose. Application of a positive lower bound may reduce maximal value of D. In one run of the model, for U_c = 0.6 mg/ℓ , $\overline{S}$ = 5000 lb/day, D reduced from 28034.4 lb/day to 25306.5 lb/day as $\underline{S}$ was increased from 0 to 1000 lb/day. The concentration profile and the optimal discharge plan for $\underline{S}$ = 500 lb/day is presented as No. 1 in Table XI.



U_c = 0.4 mg/liter

$\overline{S}$ = 1500 lb/day

FIGURE 10. OPTIMAL DISCHARGE PLAN AND CONCENTRATION PROFILE

TABLE XI

EFFECTS OF LOWER BOUND ON S_i AND NONUNIFORM UPPER BOUND ON CONCENTRATION

No.			Section No.	0	1	2	3	4	5	6	7	8	9	10	11
1	U_c = 0.6 mg/ℓ $\underline{S}$ = 500 lb/day $\overline{S}$ = 5000 lb/day	D = 28034.4	c_i mg/ℓ	.3997	.3722	.4378	.5238	.5337	.6000	.5992	.5953	.4645	.4355	.1876	0
			S_i lb/day	-	534.4	500	500	500	500	5000	5000	5000	5000	5000	5000
2	U_c = 0.6 mg/ℓ $\underline{S}$ = 0 lb/day $\overline{S}$ = 5000 lb/day	D = 28034.4	c_i mg/ℓ	.5256	.4623	.5022	.5532	.5507	.6000	.5992	.5953	.4645	.4355	.1876	0
			S_i lb/day	-	303.4	0	0	0	0	0	5000	5000	5000	5000	5000
3	$\underline{S}$ = 0 lb/day $\overline{S}$ = 5000 lb/day	D = 23611.8	U_{ci} mg/ℓ	.6	.6	.6	.6	.4	.4	.4	.6	.6	.6	.6	.6
			c_i mg/ℓ	.1997	.2019	.2272	.3153	.3056	.4000	.4000	.4513	.3654	.3519	.1580	0
			S_i lb/day	-	0	0	202.9	0	0	0	3408.9	5000	5000	5000	5000

4. Different quality standards may be prescribed for different regions of the estuary. The effects of such nonuniform standards are shown in Nos. 2 and 3 in Table XI. Compared to No. 2, U_{ci} in No. 3 has been reduced to 0.4 mg/ℓ in Sections 4, 5, and 6, the other sections having U_{ci} value of 0.6 mg/ℓ. As a result, the concentration profile for No. 3 throughout the estuary has been depressed and, except at one section, the profile is below 0.4 mg/ℓ. Maximal D has also been reduced to 23611.8 lb/day as compared to 28034.4 lb/day for No. 2.

Various other patterns of nonuniform quality standards may be studied for their effects on the optimal discharge plan and resulting concentration profile. Such information may be valuable while prescribing rational quality standards.

INTEGRATED DISPERSION AND TREATMENT MODEL

The Integrated Dispersion and Treatment Model has been presented as a linear program in Chapter VII. Solution of this model provides an optimal plan for waste treatment and discharge for waste-producing agencies which minimizes the total cost of waste treatment.

The model is demonstrated in Suisun Bay. A sketch of Suisan Bay, along with the locations of outfalls of eight industrial and three municipal dischargers of effluent, is shown in Figure 11. Waste discharge data are the same as used by Carew and McGauhey [5] and are taken from Table 5-7 in [35] which gives the waste load in terms of concentration of various constituents and the daily flow of effluent in million gallons.

A treatment cost and efficiency matrix, developed by Carew and McGauhey [5, Table III] is presented as Table XII. The percentage of each of several chemical constituents of raw effluent remaining after zero to six levels of treatment is tabulated in this matrix, together with the estimated cost of treatment to each level. After secondary treatment for sewage, for example, the table shows the residual values: 10 percent of total suspended solids and of BOD, 20 percent of COD, 40 percent of phosphates, and 50 percent of nitrogen. The cost of $100 per million gallons per day represents the cost of secondary treatment. We note that application of higher levels of treatment results in lower waste residuals, but at an increased cost.

For illustrative purposes two constituents of water quality – phosphate and BOD are chosen, although the model can easily accommodate more constituents at added computational effort which is almost directly proportional to the number of constituents.

The linear programming model for a conservative constituent is represented by Equations (7-5) through (7-10) in Chapter VII, and these could be directly applied for phosphate. The d_i , g_i , and $\bar{g}_i$ values presented in Table IX will be used for phosphate. The modifications needed for a degradable constituent such as BOD is presented in Appendix A and Equation (A3) is used in place of Equation (7-4) with corresponding modifications in Equations (7-5) and (7-7). The values of the coefficients d_i and g_i presented in Table XIII are computed from the hydrological data of Table IX, and $\bar{g}_i$ is obtained by multiplying g_i by a unit conversion factor as before.

The industries and cities discharging in Suisan Bay and their daily phosphate and BOD load is tabulated in Table XIV. The code names used in the program for the dischargers is shown in parenthesis. The values of coefficients $a_{k,\ell,m}$ for the above dischargers have been computed and tabulated in [5, Appendix B] for ten industrial constituents including phosphate and BOD. These have been computed from waste load information using the cost and treatment efficiency matrix. We note that the coefficients $a_{j,k,\ell,m}$ in our model are the same as $a_{k,\ell,m}$ in [5]. In the linear program, the variables $x_{j,k,\ell}$ have coefficients $b_{i,j,k,\ell,m}$ which are obtained by multiplying $a_{j,k,\ell,m}$ by the corresponding value of g_i according to Equation (7-11). For example,

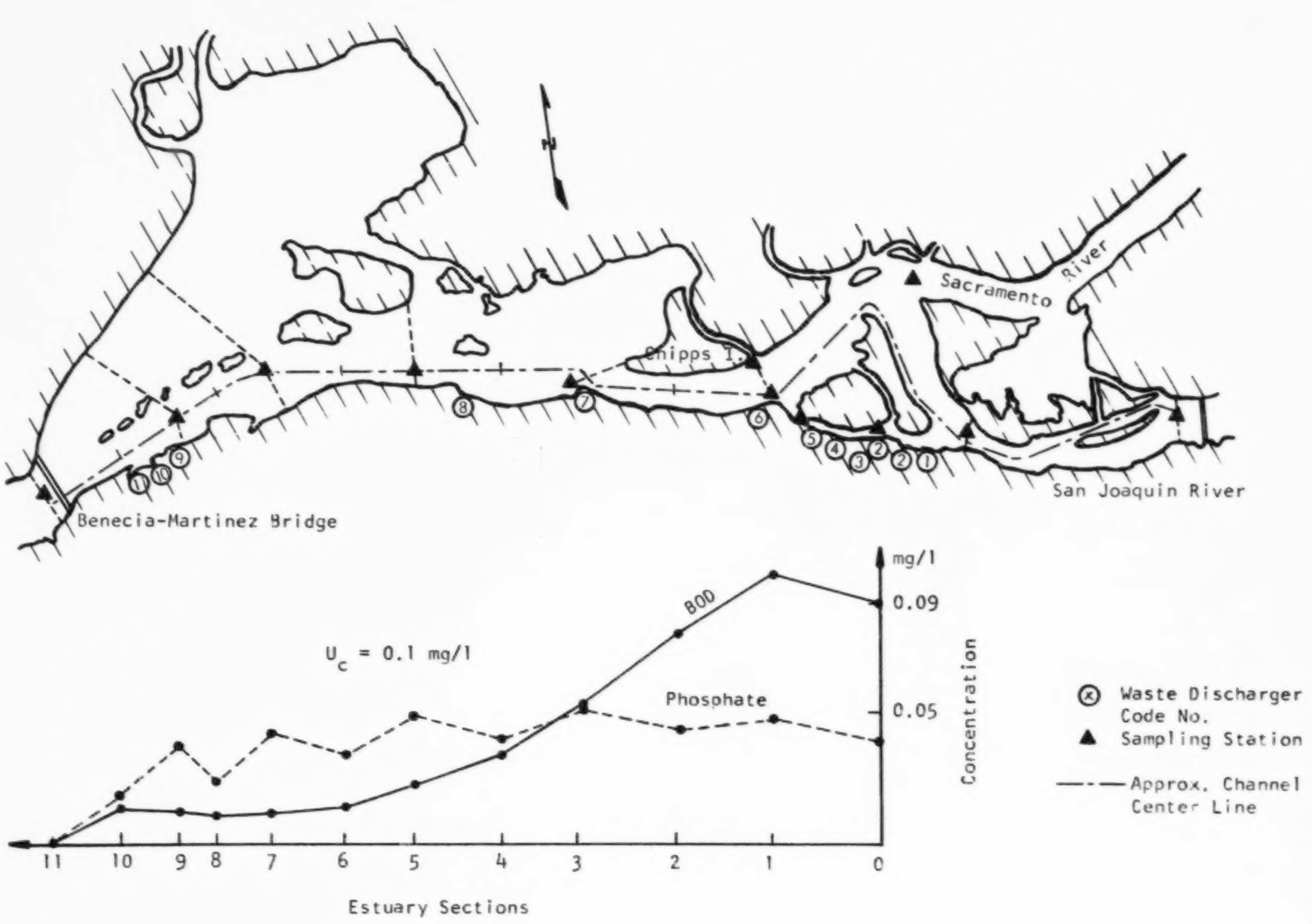

Sacramento River
Chipps I.
San Joaquin River
Benecia-Martinez Bridge
N
1
2
2
3
4
5
6
7
8
9
10
11
mg/l
0.09
0.05
BOD
Phosphate
U_c = 0.1 mg/l
Concentration
Estuary Sections
11
10
9
8
7
6
5
4
3
2
1
0
⊗ Waste Discharger Code No.
▲ Sampling Station
—·— Approx. Channel Center Line

FIGURE II. SUISUN BAY

TABLE XII

COMPOSITE TREATMENT COST AND TREATMENT EFFICIENCY MATRIX

(Coefficients of Amount of Characteristic Remaining
After Each Treatment 0, 1, 2, 3, 4, 5, 6)

Characteristic	Treatments[a]						
	0	1	2	3	4	5	6
1. Costs, Dollars per mgd[b]	0	30	100	180	280	430	540
2. Total Sulfide	1.00	0.80	0.62	0.40	0.10	0.05	0.01
3. Settleable Solids	1.00	0.40	0.02	0.01	0.01	0.01	0.01
4. Volatile Suspended Solids	1.00	0.60	0.40	0.24	0.05	0.01	0.01
5. Total Suspended Solids	1.00	0.50	0.10	0.08	0.01	0.01	0.01
6. Biochemical Oxygen Demand	1.00	0.60	0.10	0.07	0.07	0.01	0.01
7. Chemical Oxygen Demand	1.00	0.70	0.20	0.15	0.15	0.01	0.01
8. Chloride	1.00	0.60	0.10	0.07	0.07	0.01	0.01
9. Phenol	1.00	0.70	0.12	0.10	0.07	0.05	0.01
10. Oil and Grease	1.00	0.70	0.62	0.13	0.07	0.05	0.01
11. Cadmium	1.00	0.70	0.25	0.10	0.05	0.01	0.01
12. Chromium	1.00	0.70	0.30	0.10	0.05	0.01	0.01
13. Copper	1.00	0.80	0.20	0.10	0.05	0.01	0.01
14. Lead	1.00	0.70	0.10	0.10	0.05	0.01	0.01
15. Zinc	1.00	0.70	0.40	0.10	0.05	0.01	0.01
16. Dissolved Silica	1.00	0.70	0.40	0.10	0.05	0.01	0.01
17. Phosphate	1.00	0.90	0.40	0.10	0.05	0.05	0.01
18. Nitrogen	1.00	0.90	0.50	0.50	0.50	0.45	0.25

[a] The treatment corresponding to the columns numbered 0 through 6 are as follows:
0 Zero treatment
1 Conventional primary
2 Conventional secondary
3 Lime-alum coagulation, sedimentation, and rapid sand filtration
4 Adsorption
5 Electrodialysis
6 Evaporation

[b] Million gallons daily.

TABLE XIII

COEFFICIENTS FOR DISPERSION MODEL WITH DEGRADABLE CONSTITUENTS IN SUISUN BAY

Section No. i	d_i	g_i 10^{-4}	$\bar{g}_i$ 10^{-4}
0	1.1212	0.807	0.14883
1	1.1183	0.790	0.14563
2	1.2175	1.181	0.21752
3	1.1546	1.050	0.19355
4	1.1277	0.898	0.16553
5	1.1377	1.090	0.20093
6	1.0933	0.730	0.13457
7	1.0728	0.627	0.11558
8	1.0501	0.440	0.08111
9	1.0624	0.550	0.10139
10	1.0607	0.540	0.09954
11	-0.9572	0.380	0.07005

$$\left.\begin{aligned} d_i &= 1 + \frac{v_i x_{i+1}}{E_i} \\ g_i &= \frac{x_{i+1}}{A_i E_i} \\ \bar{g}_i &= 0.1843\ g_i \end{aligned}\right\} \quad i = 0, 1, \ldots, n-1$$

$$d_n = \frac{x_n v_n}{E_n} - 1$$

$$g_n = \frac{x_n}{A_n E_n}$$

$k = 0.17/\text{day}$

$n = 11$

TABLE XIV

MAJOR DISCHARGERS IN SUISUN BAY – LOCATION AND CONSTITUENT LOAD

Reach	No.	Industry or City	Phosphate lb/day	BOD lb/day
1	1	Ethyl Corporation (ETL)	0.14	0.4
1	2	Dow Chemical Company (DOW)	2.30	18.0
1	3	H. K. Porter Company (HKP)	0.15	1.80
1	4	U. S. Steel Corp. (USS)	1.60	235
1	5	John Mansville Products Corp. (JMP)	0.43	>172
2	6	City of Pittsburg (COP)	586	1346
3				
4	7	Shell Chemical Company (SHL)	11.0	143
5	8	Allied Chemical Corp. (ACC)	0.6	<6
6				
7				
8				
9				
10	9	Tidewater Oil Company (TOC)	6.9	1772
10	10	City of Concord (COC)	277	484
10	11	Central Contra Costa Sanitary District (CCD)	3031	6048
11				

a_{111}, the coefficient for Ethyl Corporation, treatment 1 and component 1 (phosphate), is given in [5] as 0.04. To obtain b_{3111} a coefficient for the variable ETL1, 0.04 is multiplied by 0.3798×10^{-4}, the value of $\bar{g}_3$, to obtain 0.01519×10^{-4} . Equation (7-8) assures that the total effluent load $d_{j\ell}$ is taken care of for each discharger.

The resulting linear program has 60 rows and 125 columns, including the slack variables and 24 rows for upper bounds on concentrations. Once the basic linear programming tableau is ready, the model may be applied to answer various questions by changing the right-hand constants for varying the upper bounds on concentration and/or waste loads.

Initially the model was used for only one constituent – phosphate – and the maximum allowable concentration U_c was varied from 0.5 mg/ℓ to 0.05 mg/ℓ. At U_c = 0.5 mg/ℓ, only the treatment processes COP2, COP3, and CCD2 are used. But as the quality standard is tightened more costly treatment processes are used.

At U_c = 0.05 mg/ℓ, JMP3, COP6, COC3, CCD3, and CCD4 are used. We note that while City of Pittsburg is using treatment 6, some other industries are still not treating their wastes, as this is economical for the region. Table XV below presents the total treatment costs for different values of U_c .

TABLE XV

VARIATION OF TOTAL COST WITH CHANGES IN
U_c FOR PHOSPHATE

U_c in mg/ℓ	0.5	0.4	0.3	0.2	0.1	0.05
Total Cost in $	575	836	1098	1547	2312	3646

The same upper bound on concentration, U_c = 0.1 mg/ℓ was used both for phosphate and BOD and the resulting concentration profiles for phosphate and BOD are shown in Figure 11 below the sketch of the estuary.

The effect of tightening the quality standard to U_c = 0.05 mg/ℓ for both phosphate and BOD on total cost and optimal plan of treatment is presented in Table XVI. It is seen that now all the industries are treating their wastes which was not the case for ETL, DOW, HKP, and ACC for U_c = 0.1 mg/ℓ, and the total cost has increased by $4998.

On further tightening of the quality standard to U_c = 0.03 mg/ℓ for both phosphate and BOD, the problem became infeasible and it was observed that even with most of the industries treating at 6th level of treatment at a total cost of $39,366, the quality standard could not be met.

It is seen that for U_c = 0.1 mg/ℓ, the concentration profile for BOD reaches this maximum level at section 1, but the maximum concentration of phosphate is

TABLE XVI

OPTIMAL TREATMENT PLANS FOR DIFFERENT QUALITY STANDARDS

Waste Discharger	Effluent Output mgd	Type of Treatment Recommended	
		U_c = 0.1 mg/ℓ	U_c = 0.05 mg/ℓ
ETL	0.46	0	1
DOW	27.60	0	0-(4.46) & 2-(22.14)
HKP	0.89	0	2
USS	18.70	0-(16.11) & 2-(1.59)[a]	0-(6.86) & 2-(11.84)
JMP	1.04	5	5
COP	1.58	5	5
SHL	13.00	2	2
ACC	3.80	0	2
TOC	41.50	3-(5.51) & 5-(35.99)	5
COC	3.10	5	5
CCD	8.26	5	5
Total Cost	-	$24039	$29037

[a] We note a combination of zero treatment and second level of treatment is more economical than first level of treatment here.

0.05038 mg/ℓ at section 3. So U_c for phosphate could be lowered to this value without increasing the total cost. In maintaining the required quality standard for BOD, the treatment processes remove more phosphate than needed and there is spare capacity for phosphate.

The effects on total cost and optimal plan of treatment of increasing the effluent load of the waste dischargers is presented in Table XVII. Such an increase in effluent load is expected with industrial and population growth in the future. For $U_c = 0.1$ mg/ℓ for both phosphate and BOD, the effluent loads were increased by 25 percent, 50 percent, and 100 percent.

However, when the quality standards were set at $U_c = 0.05$ mg/ℓ for both phosphate and BOD, the problem was infeasible even with a 25 percent increase in effluent load. Even with most of the industries using high levels of treatment at a total cost of $35,717, the quality standard could not be met.

DISCUSSIONS

In the illustration of the water quality control model, only two quality factors were considered. However, the model is general and only computational effort and cost are the limitation to the number of constituents that could be considered. Although the example herein involves some arbitrary quality standards, this seems to be a valid approach which might be utilized in policy decision-making based on quality-cost relations. The decision to achieve water quality standards at a minimum cost for the region may be an important step toward removing the "technological external diseconomies" [1] and achieving optimal allocation of resources. It is true that a jurisdictional arrangement is required under which the cost of treatment assessed against each discharger is independent of the degree of treatment imposed on him, but it should reflect his contribution to the waste discharged in the estuary. However, this should benefit all, including the society at large. The method may be used in predicting the future treatment needs as well, as illustrated here.

TABLE XVII

OPTIMAL TREATMENT PLANS FOR INCREASING EFFLUENT LOAD

Waste Discharger	125% Present Effluent Load mgd	Optimal Treatment Plan	150% Present Effluent Load mgd	Optimal Treatment Plan	200% Present Effluent Load mgd	Optimal Treatment Plan
ETL	0.58	0	0.69	0	0.92	1
DOW	34.50	0	41.40	0	55.20	0-(19.67); 2-(35.53)
HKP	1.11	0	1.34	0	1.78	2
USS	23.40	0-(14.81); 2-(8.59)	28.00	0-(13.55); 2-(14.45)	37.40	0-(13.26); 2-(24.14)
JMP	1.30	5	1.56	5	2.08	5
COP	1.98	5	2.37	5	3.16	5
SHL	17.20	2	19.50	2	26.00	2
ACC	4.80	0	5.70	0	7.60	2
TOC	51.90	3-(5.45); 5-(46.45)	62.20	3-(1.52); 5-(60.68)	83.00	5
COC	3.90	5	4.60	5	6.20	5
CCD	10.32	5	12.39	5	16.52	5
Total Cost		$31058		$38755		$57245

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